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

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CFDRC

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Project ID: FC_36_Cole
Overview

- **Timeline**
  - Start Date: 6/1/07
  - End Date: 5/31/11
  - Percent Complete: 44%

- **Budget:**
  - Total Project Funding:
    - DOE $4,900K
    - Contractors $1,500K
  - Funding Received in FY08
    - $1,175K
  - Funding for FY09
    - $780K

- **Barriers:**
  - D. Water Transport within Stack
  - E. System Thermal and Water Management
  - G. Start-up and Shut-down Time and Energy / Transient Operation

- **Transportation Stack Targets**
  (2005 status / 2010):
  - Stack power density, W/L: (1500 / 2000)
  - Cold start-up time to 50% rated power @ -20°C, secs: (<10 / 5)

- **Partners:**
  - Ballard Power Systems
  - BCS Fuel Cells
  - ESI Group, NA
  - Techverse
  - U. Victoria
  - SGL Carbon
Program Objectives => Relevance

- **Overall:**
  - Improve understanding of the effect of various cell component properties and structure on the gas and water transport in a PEM fuel cell;
  - Demonstrate improvements in water management in cells and short stacks; and
  - Encapsulate the developed understanding in models and simulation tools for application to future systems.

- **FY 2008 and 2009:**
  - Complete baseline characterization for Gas Diffusion Layer (GDL) materials
    - Key fundamental properties affecting water transport
  - Gather experimental data under controlled conditions, test and apply models for water transport in GDLs, channels, and across interfaces
    - Improved understanding of water transport, initial screening of improvement concepts to remove water and/or control its distribution
  - Evaluate performance and water management sensitivity in operational cells, evaluate cell-scale water transport models on component level, integrate with electrochemistry and test
    - Data and tools for screening of concepts to improve water management while increasing power densities, mitigate liquid-water induced pressure drops and transients for system-level benefits
**Approach**

**Experimental Characterization**

- Advanced Model Development (CFD/LBM)
  - LBM models for microscale flow thorough porous media: in-plane and through-plane permeabilities, capillary pressure, and wetting characteristics
  - CFD models for macroscopic two-phase flow in channels, GDLs and interfaces, coupled with electrochemical reaction and transport through membrane

Simulations of gas, water and thermal transport in a unit cell complement experiments to develop understanding, evaluate concepts

- Ex-situ characterization: key materials properties and sensitivity to treatments, water transport analysis in GDLs and micro-channels
- In-situ diagnostics: current and water distribution

Provides fundamental understanding, validation data for physics-based models from component to cell level

**Multiphysics Modeling**

- Cell flooding sensitivity to materials and operating strategies
- Implement and test performance improvement strategies

Improved component designs and operating strategies, tools for addressing water transport in future generation designs

**Improved Water Management Through Improved Component Designs and Operating Strategies**

**Improved Component and Fuel Cell Concepts**
### FY08-09 Plans and Milestones

<table>
<thead>
<tr>
<th>Month/Year</th>
<th>Milestone</th>
<th>Comments</th>
<th>% Complete</th>
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<tbody>
<tr>
<td>May 08</td>
<td>Ex-situ GDL materials characterization</td>
<td>Two-phase transport data limited, needs further analysis</td>
<td>100 %</td>
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<tr>
<td>Dec 08</td>
<td>GDL-Channel water transport experimental characterization</td>
<td>Initial data on model systems, GDL data delayed for increased channel studies</td>
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<tr>
<td>May 09</td>
<td>LBM microscale model for two-phase flow</td>
<td>Development complete, testing and application underway</td>
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<tr>
<td>Jun 09</td>
<td>Cell-scale water transport model implemented, component models validated</td>
<td>Ongoing, initial numerical issues resolved and experiments underway for channels. GDL-channel interface experiments and model treatment lagging</td>
<td>75%</td>
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</table>
Key property database established for SGL, BMP & Toray papers with a range of PTFE loadings (Ballard, Techverse):

- Porosity and Pore Size Distribution (MIP, MSP)
- In- and Through-Plane Gas Permeability, Effective Diffusivity
- Electrical and Thermal Conductivity
- Thickness & Electrical Resistance Variation with Compression
PTFE Effects on Gas Transport

Ballard Laser Scans

PTFE 0%  
PTFE 20%  
PTFE 40%

Laser scan images of Toray-050, Ballard Power Systems

Numerically Generated Microstructures for LBM

PTFE distribution model developed from measured pore size distributions, laser scan images, and processing observations:
- Teflon® solution is hydrophilic to carbon fibers.
- Small pores and corner of larger openings are filled first.
- Increase in fiber diameter due to Teflon® coating is negligible.

PTFE distribution model developed from measured pore size distributions, laser scan images, and processing observations:

Validates LBM for gas phase transport in GDL materials
Verifies simple, stochastic microstructure generation approach is adequate for analysis of transport, PTFE loading effects in carbon paper GDLs
IPP approximately linear in PTFE loading and porosity to 30% loading
Capillary Pressure and Residual Saturation

- Positive Water Displacement technique, 90 mm diameter media for greater resolution

- Techverse quantified breakthrough and residual saturation by volumetric and gravimetric analysis;
  - PTFE loading reduces saturation at breakthrough, not residual

- Addition of PTFE backing brings PC measurements closer to other reported ranges

- Greater hysteresis effect with increasing Teflon® content of media, weaker effect in Toray with no MPL
Capillary Pressure Simulation

- Toray-050
  - (a) $\alpha = 0.3$, dispersed globules
  - (b) $\alpha = 0.4$, interconnected streams
  - (c) $\alpha = 0.7$, droplet emergence

Hydrophobic porous plug to prevent liquid escape from GDL.

$\alpha = 0.7$

- Similar model definition, with water reservoir and hydrophobic ‘frit’, used to verify capillary pressure implementation in CFD-based two-fluid code
- LBM Results guided implementation details in CFD continuum model
Gas Permeability in Wet Media

- Analysis ongoing to quantify saturation level and extract relative permeability
- No significant difference between initially humidified and dry gas
- PTFE loading did not significantly alter the behavior for SGL materials with MPL

Water Permeability

- Increasing PTFE content reduced water permeability
- Three distinct flow regimes.
  - 1: No flow. (below breakthrough pressure)
  - 2: Constant permeability. (moderate pressure)
  - 3: Increase in permeability with increased pressure, indicating opening of more channels for water flow
Transient GDL Water Transport Characterization and Modeling

UVic is *Simultaneously* monitoring the development of the capillary flow, pressure, and volume injection rate of water percolating through the GDL porous layer.

**LBM Modelling of GDL Transport**

- Qualitative agreement, insight into under-surface transport
- Experiments and LBM guiding CFD model improvements

Image analysis quantifying cluster and droplet growth dynamics near/on surface

Dry sample: first breakthrough
Previously wet sample: continuous loading test

Invasion depends on history
Droplet Emergence Analysis

Time evolution of droplet emergence images

PDMS Chip and droplet dynamics studies at UVic for channel/GDL interface model

- Image analysis for temporal correlation and FFT to quantify droplet emergence frequency

Experimental conditions:
- Inlet pressure, $P_0$: 16.34 psia
- Squared water pore size, $d_{w}$: 50 um
- Squared gas microchannel, $d_{A}$: 250 um
- Water injection speed, $V_w$ (cm/sec): 4 cm/s
- Air velocity, $V_A$: 10 m/s
- Re$_A$: 164, Bo: 3.36E-4, Ca: 5.50E-4

Initial Model Tests: Film/mist formation from drag overcomes surface tension
Ballard Two Phase Flow Channel DP Measurement

- Interchangeable single channel graphite plates
- Nineteen pressure taps spaced 1.5cm apart (27cm total measurable length)
- Two phase pressure drop measured between taps 1 and 19 and water injected from tap 2
## Two Phase Channel Model Validation Test Matrix

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<td>11</td>
<td>20</td>
<td>1.013</td>
<td>61, 204, 306, 407</td>
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<td>75</td>
<td>20</td>
<td>1.013</td>
<td>61, 204, 306, 407</td>
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</tbody>
</table>

### Experimental error estimation

Keyence microscope assessment of micro-channel machining accuracy (within 10 μm)

- **Baseline**
  - 407 sccm, 37 mL/min

- **Design 2**
  - 0.98
  - 80.0°
  - 0.31
  - 80.0°
CFD Pressure Drop Validation with Water Flow Rate

- Steady two-phase CFD captured trends with water flow rate
- Experimental repeatability worse at low water and low air

(Teflon Film as the Seal: 61SCCM)

(Teflon Film as the Seal: 407SCCM)
CFD underpredicts measured pressure drop variation with total flow:

- Better interfacial drag models needed for PEMFC relevant flows and channel sizes, means to capture wall film effects with practical grid resolution
- Further investigation in liquid water injection variability being carried out
Stratified, Wavy Flow Verification

- ESI achieved qualitative agreement with experiment for slug behavior in a stratified two-phase channel flow (0.69 m/sec water, 2.2 m/sec air, 50x250 mm)
- Requires transient to capture dynamics, investigating approaches to reduce computational expense

Lower gas velocities transfer less momentum to the water, film falls to bottom due to gravity
Cell Level Water Transport Characterization

Overall Approach

- **Design Sensitivities**
  - Number of Channels (coupled channel width and depth)
  - Landing Width
  - Plate Water Contact Angle
  - Rounded vs. Angled Corners
  - Channel Pattern (i.e. straight vs. serpentine)
  - Serpentine Type (e.g. classic, parallel, separated)

- **Water Removal Concepts**
  - Gravity
  - Capillary/Surface Tension
  - Drag/Shear
  - Pressure/Momentum

- **Operating Conditions**
  - Current Density
  - Stoic
  - RH
  - Temperature
  - Pressure
  - Fluid Composition (air, hydrogen, reformate)

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Model Validation

- **Measurables**
  - **Single Cell** Pressure Drop Frequency - Ideal is Infinity
  - **Single Cell** Pressure Drop Amplitude - Ideal is Zero
  - Stack and Single Cell Ratio of Operational to Non-Operation Pressure Drops - Ideal is 1.0
  - Stack Level Confirmation

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**Validated Model**

- **Results**
  - Robust fuel cell stack capable of managing liquid water at lower pressure drops.
  - Improved system efficiencies.
  - Reduced system costs.
Water Removal and Pressure Signature

- Ideal Frequency is Infinity
- Ideal Amplitude is 0 - no change of pressure drop over time due to liquid water

Plate 1
Pressure Drop vs. Time

Plate 4
Pressure Drop vs. Time

- Operating cell pressure drop signatures for plate 1 (left) and plate 4 (right) (identical scales, different color curves represent different runs)
  - The dry pressure drops for these two plates are nearly identical
  - Plate 1 is very unstable while plate 4 runs well due to its better water management characteristics, less variation of pressure signature

<table>
<thead>
<tr>
<th>Plate</th>
<th>Pressure Drop Amplitude Relative to Plate 1</th>
<th>Pressure Drop Frequency (Hz)</th>
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<tr>
<td>1</td>
<td>1.0</td>
<td>~6e-4</td>
</tr>
<tr>
<td>4</td>
<td>0.27</td>
<td>~15e-4</td>
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- Pressure signature and water removal for different cell designs are inter-linked, signature provides a quantification of water management characteristics
- Cell level CFD modeling with validated interface drag models at channel level, validated two phase models for GDL flow and validated channel/GDL interface model is the next step
Effects of PTFE content in micro-porous layer in GDL and temperature on cell performance

- BCS Fuel Cells is evaluating the effect of hydrophilic/ hydrophobic characteristics of MPL on the catalyst side in MEAs for self-humidified fuel cells that can be operated at higher temperatures.
- Demonstrated performance sensitivity: MEA developed with 20% Teflon® in the MPL layer of carbon cloth type GDL is better than both the commercial and 5% Teflon® content MEAs operated at 60 °C and 1.75 air stoichiometry.
- GDL modifications allow effective operation at higher temperatures, and consequently increased power density, without external humidification.
Techverse will characterize water permeation through GDLs into a BCS serpentine channel design bipolar plate.

Experimental data for water leaving channels, pressure signals, and water distribution will provide additional sensitivity information and model validation.

Preliminary modeling results for a single-bend section of the plate:
- Highest channel water content, lowest water flux into channels is near outlet due to higher channel pressure as expected.
- ‘Tumbling’ flow in the serpentine corners.
- Transient simulation required for numerical stability.
Future Work and Milestones

FY09-10 Plans:

- **Characterization and Diagnostics**
  - Complete GDL-channel transport experiments

- **Model Development/Testing**
  - Complete integration of heat transfer and electrochemistry with two-phase CFD models
  - Cell-scale model evaluation against steady and transient data

- **Water Management Improvement**
  - Concept development and screening:
    - Component interaction and flooding sensitivity studies for performance improvement
    - Channel design, surface finish, and GDL design for effective removal with low pressure drop

Upcoming Milestones:

- Cell Scale model test/validation against operational cell data completed Dec 2009
- Improvement concept screening complete March 2010, optimization underway
Collaborations

- **Partners**
  - Ballard Power Systems: Measurement tools, material data, and operational test results to validate and support the development of models for water transport and management
  - BCS Fuel Cells: Operational cell and stack diagnostics, materials sensitivity and serpentine channel design
  - ESI Group, NA: Model implementation and software integration, model testing
  - Techverse: Materials characterization, ex-situ water transport
  - SGL Carbon: GDL and bipolar plate materials
  - U. Victoria: GDL permeation, channel droplet injection and transport quantification

- **Technology Transfer**
  - Univ. of South Carolina NSF I/UCRC Center for Fuel Cells: Presented overview of this work, beneficial follow-on discussions on model formulation, material characterization
Summary

- **Relevance:**
  - Effective water management is necessary to improve automotive fuel cell performance, freeze/thaw cycle tolerance, and cold startup times

- **Approach:**
  - Integrated characterization and model development to advance understanding, application of the resulting knowledge to optimization

- **Technical Accomplishments and Progress:**
  - Completed characterization of key physical and transport properties for SGL, BMP and Toray GDL materials
  - Validated multiphase LBM applied to analyze impact of microstructure and Teflonation on permeability, wetting characteristics and breakthrough, and capillary pressure behavior; Also guiding model developments for continuum CFD
  - Implemented experimental setup for collecting wet pressure drop and transient pressure signatures in two-phase flows in channels and cells; Data being used for CFD model development and validation
  - Started gathering experimental data for droplet emergence at GDL-channel interface; currently being used in model development
  - Demonstrated sensitivity of cell operation to water management through materials and design modifications
  - Began integration of electrochemistry, heat transfer, and phase change with the CFD two-phase flow models

- **Proposed Future Work:**
  - Complete GDL-channel transport experiments and channel/cell pressure signature measurements for different channel types and surface finish
  - Complete integration of electrochemistry, heat transfer and phase change models with two-phase CFD models; Test and validate the developed integrated models using operational cell-scale steady and transient data
  - Apply validated measurements and simulation tools to identifying optimization strategies: Channel design, surface finish, and GDL design for effective removal with low pressure drop