Delivering Breakthrough Solutions

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

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CFD Research Corporation

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Project ID: FC030

Overview

- **Timeline**
  - Start Date: 6/1/07
  - End Date: 5/31/11
  - Percent Complete: 70%
- **Budget:**
  - Total Project Funding:
    - DOE $4,900K
    - Contractors $1,500K
  - Funding Received in FY09
    - $1,000K DOE
    - $402K Cost Sharing by Team
  - Funding for FY10
    - $1,175 K DOE
- **Barriers:**
  - D. Water Transport within Stack
  - E. System Thermal and Water Management
  - G. Start-up and Shut-down Time and Energy / Transient Operation
- **Partners:**
  - Ballard Power Systems
  - BCS Fuel Cells
  - ESI Group, NA
  - Techverse
  - U. Victoria
  - SGL Carbon

Program Objectives => Relevance

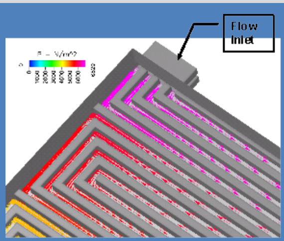
- **Overall:**
  - **Improve understanding of the effect of various cell component properties and structure on the gas and water transport in a PEM fuel cell;**
  - **Demonstrate improvements in water management in cells and short stacks; and**
  - **Encapsulate the developed understanding in models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

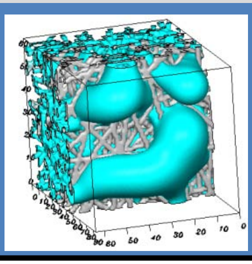
- **FY 2009 and 2010:**
  - **Gather experimental data under controlled conditions, test and apply models for water transport in GDLs, channels, and across interfaces**
    - **Improved understanding of water transport, initial screening of improvement concepts to remove water and/or control its distribution**
  - **Evaluate cell-scale water transport models on component level, integrate with electrochemistry and heat transfer, test and apply for operational cells**
    - **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**
  - **Develop and screen concepts for water management improvement**
    - **Component interaction and flooding sensitivity studies for performance improvement**
    - **Channel design, surface finish, and GDL design for effective water removal with low pressure drop**

Approach

Improved Water Management Through Improved Component Designs and Operating Strategies

Advanced Model Development (CFD/LBM)

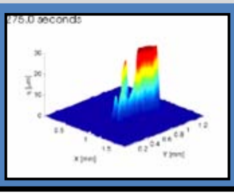


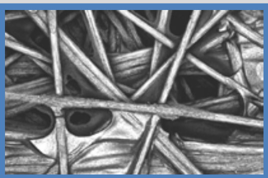


- **LBM models for microscale flow thorough porous media: in-plane and through-plane permeabilities, capillary pressure, and wetting characteristics**
- **CFD models for macroscopic two-phase flow in channels, GDLs and interfaces, coupled with electrochemical reaction and transport through membrane**

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

Experimental Characterization



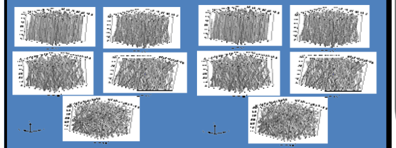


- **Ex-situ characterization: key materials properties and sensitivity to treatments, water transport analysis in GDLs and micro-channels**
- **In-situ diagnostics: current and water distribution**

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

Improved Component and Fuel Cell Concepts

Thickness	Density: high	Density: low	
200 µm/8 mil	GDL 24	GDL 25	2 D - paper
300 µm/12 mil	GDL 34	GDL 35	2 D - paper
400 µm/16 mil		GDL 10	3 D - nonwoven



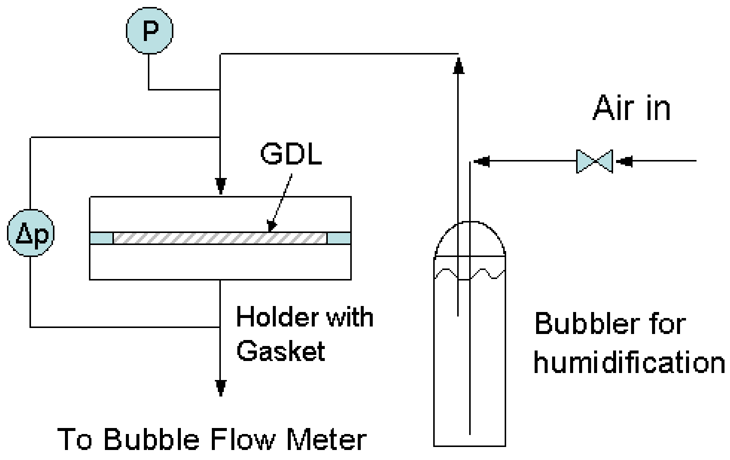
- **Cell flooding sensitivity to materials and operating strategies**
- **Implement and test performance improvement strategies**

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

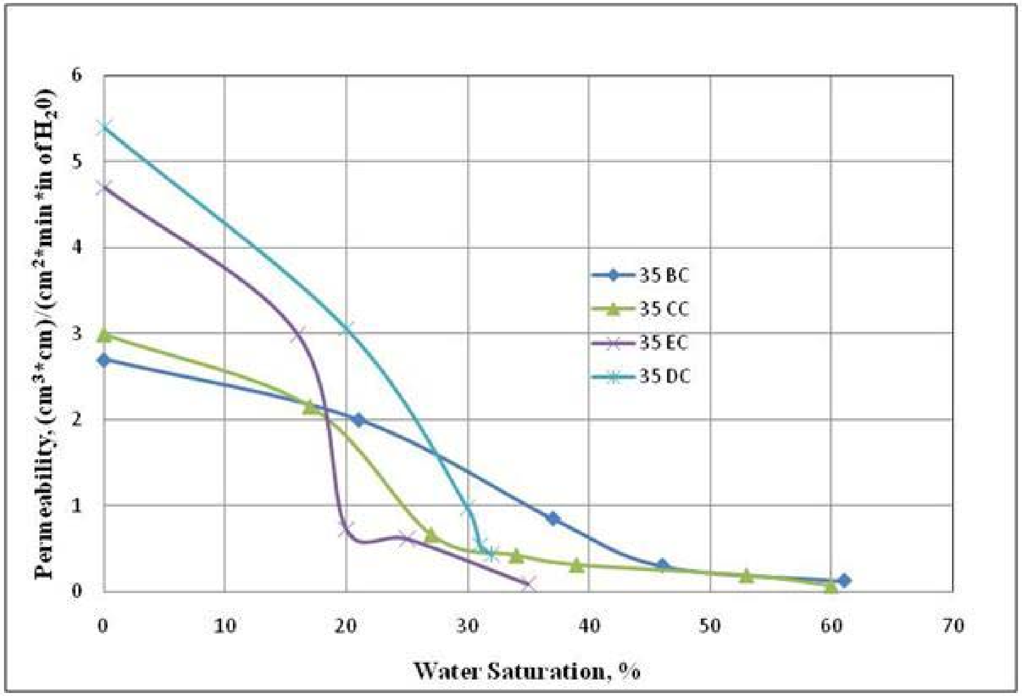
FY 09-10 Plans and Milestones

Month/Year	Milestone	Comments	% Complete
Dec 08	GDL-Channel water transport experimental characterization	GDL data delayed for increased channel studies, now complete	100%
Jun 09	Cell-scale water transport model implemented, component models validated	Ongoing challenges in matching experimental data for dP variation at low air flows and/or liquid water fractions	90%
Dec 09	Cell scale models with electrochemistry and heat transfer complete, validated	Heat transfer and phase change issues have delayed progress	75%
Mar 10	Water management concepts identified, screening and improvement initiated	Experimental studies are progressing at Ballard and BCS	75%

Effect of Relative Saturation on Gas TPP of GDL



Permeability Flow Apparatus

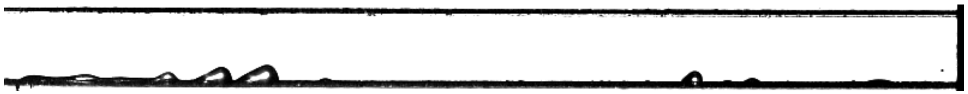


- **Techverse completed two-phase permeability studies. Gas permeability was found to increase significantly below a threshold water saturation, typically 20%, for all SGL media**
- **Permeability of the MPL layer is approximately an order of magnitude lower than the carbon paper, and dominates the through plane permeability of GDL media**

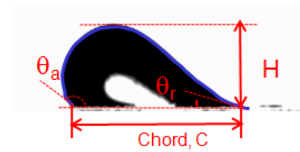
Droplet Emergence Analysis and Prediction

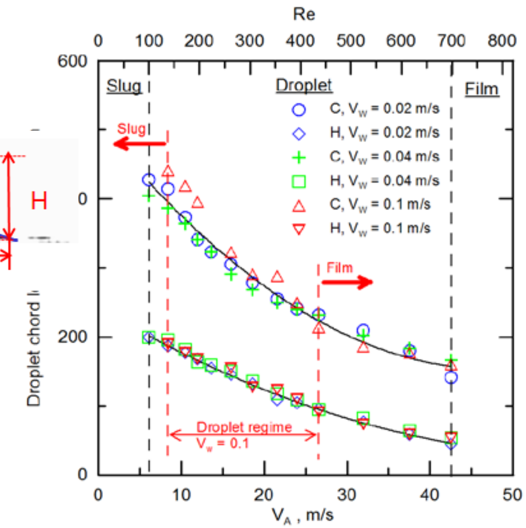
Slug Flow, V_w=0.04 m/s, V_A=4 m/s

Droplet Flow, V_w=0.04 m/s, V_A=10 m/s

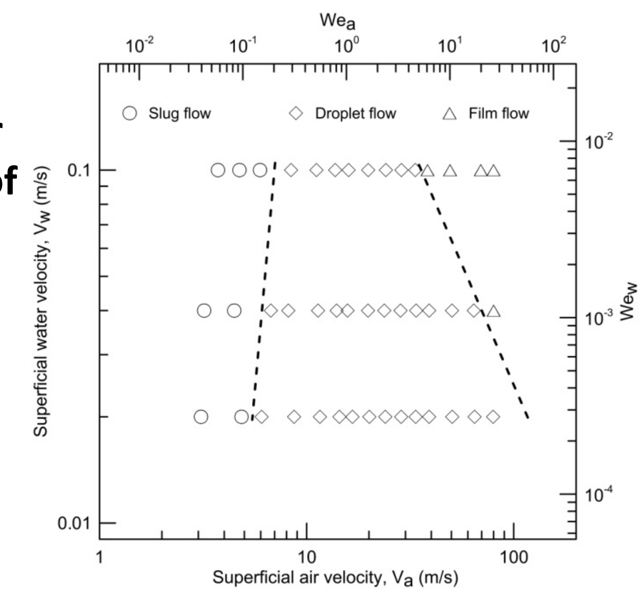


Film Flow, V_w=0.04 m/s, V_A=43 m/s



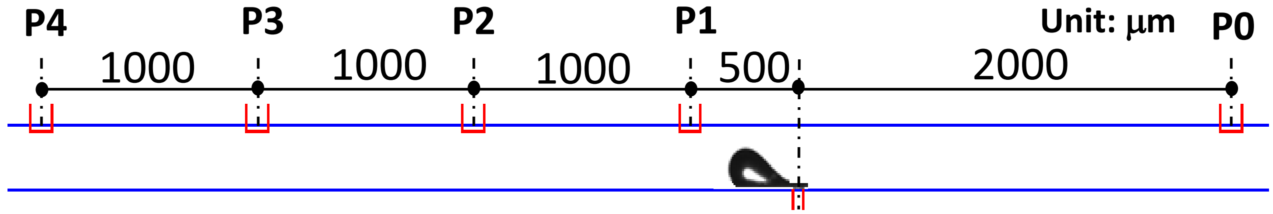


- **U. Victoria PDMS Chip droplet dynamics studies for controlled experiment mimicking water emergence at channel/GDL interface**
- **At operating conditions, droplet height is independent of water injection rate. Air velocity controls drop size and drives onset of film flow, water flow influences transition to slug and film from droplet regime**
- **With improved dynamic contact angle inputs, models capture trends in shape. Frequency improves with model length**

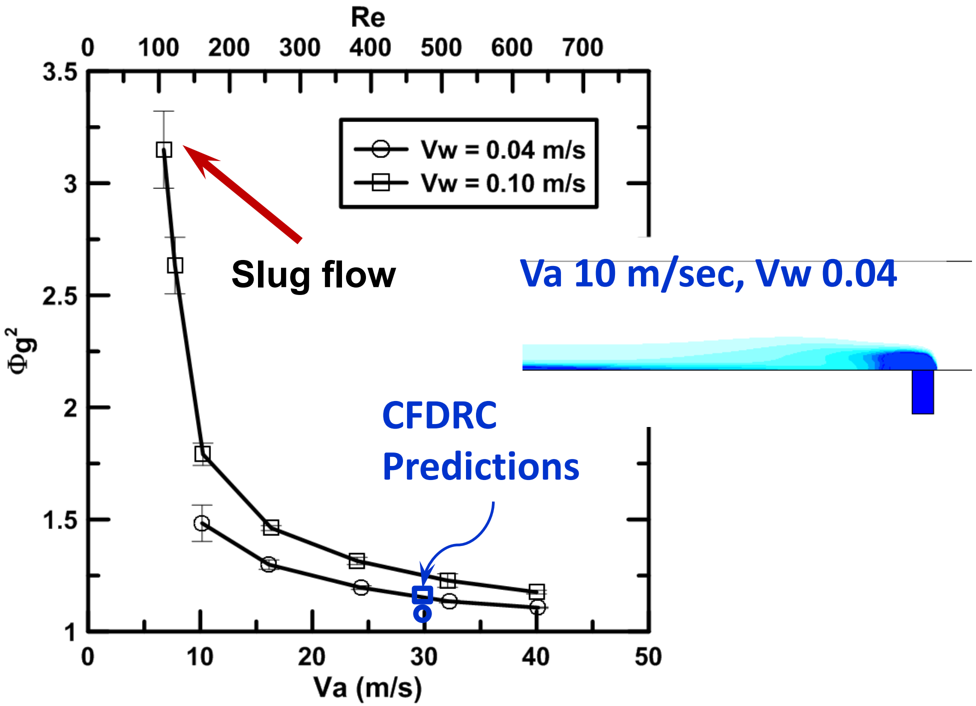


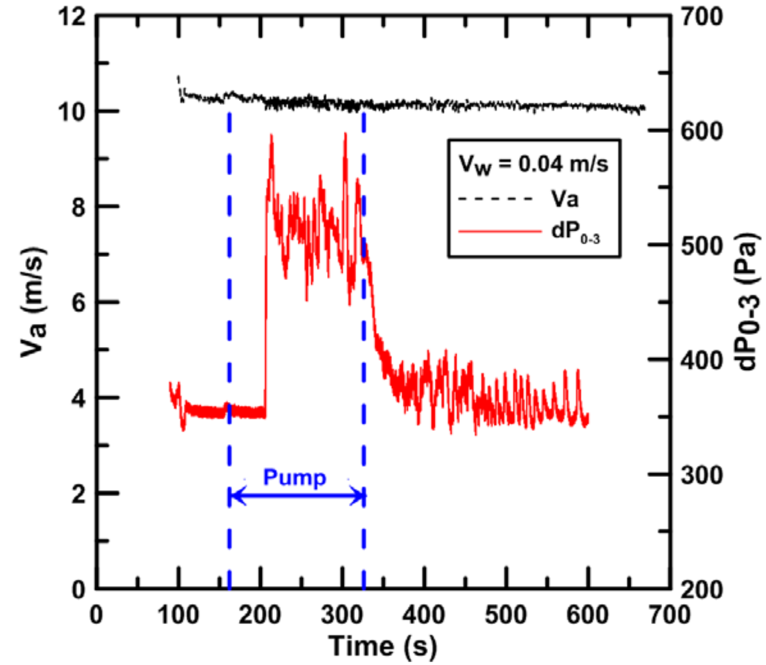
Predicted, V_w=0.04 m/s, V_A=10 m/s

Droplet Emergence Effects on Pressure Drop



Pressure drop (dP) between ports in gas channel under different air velocities

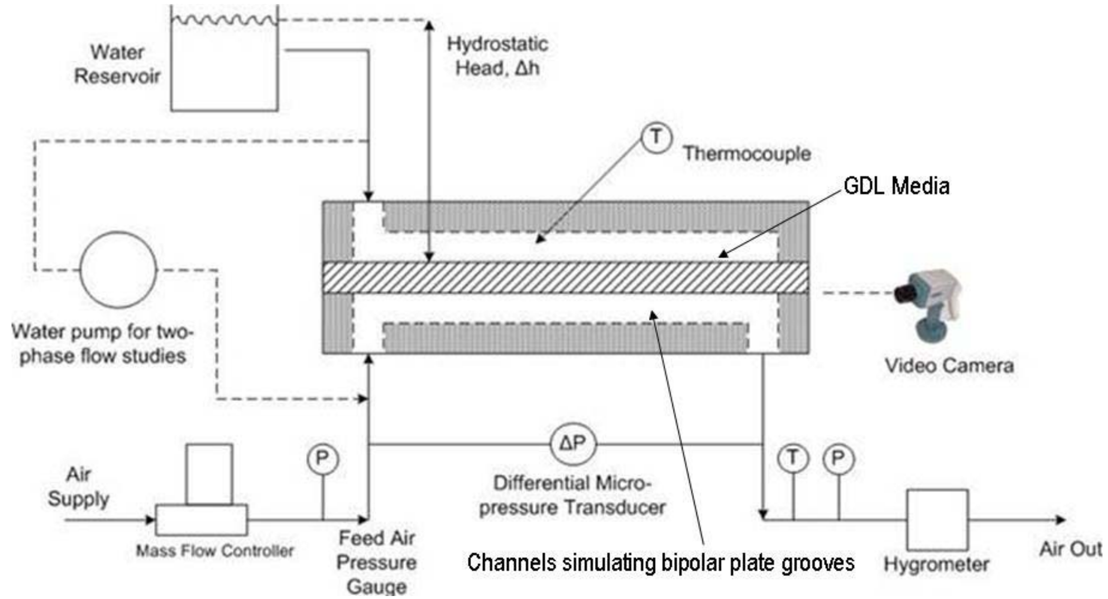




Typical differential pressure (dP_{0-3}) signal in a two-phase flow channel measure between P0 and P3.

Two Phase Flow Pressure Drop in Serpentine Bipolar Plate Channels

- Techverse examined four orientations – horizontal cell with water flowing either up or down in the GDL media, vertical cell with air flowing up or down the channels
- Horizontal cell with water above channel exhibited the least two phase flow pressure drop
- Vertical cell with air flowing up indicated the largest pressure drop for the same air/water flow rates

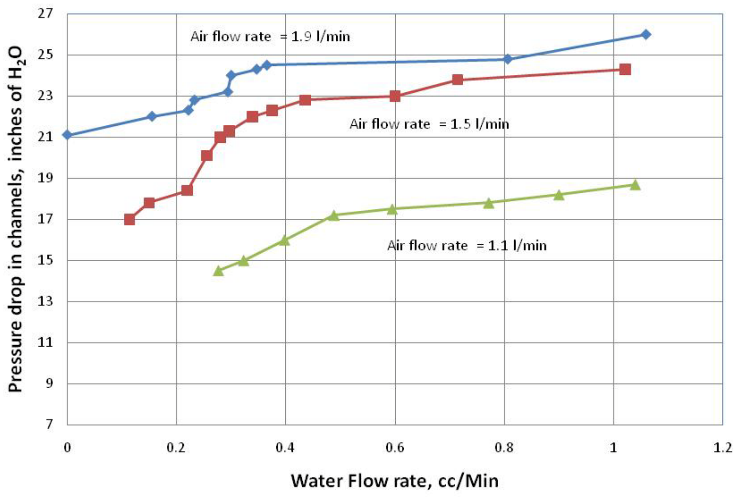


Schematic of Water Transport Visualization Apparatus

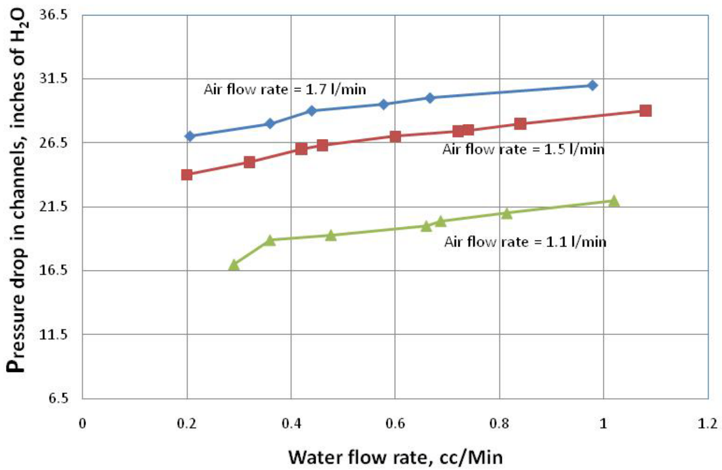
- Vertical cell orientation with air flowing down exhibited the least percentage of the wetted channels at the high water flow conditions, i.e. more GDL open area
- Configurations of horizontal cell with water flowing up and vertical cell with air flowing up are most likely to form water film blocking open GDL surface area
- Elevated temperature of 60°C had minimal effect on two phase flow pressure drop characteristics

Serpentine Wet dP: Horizontal

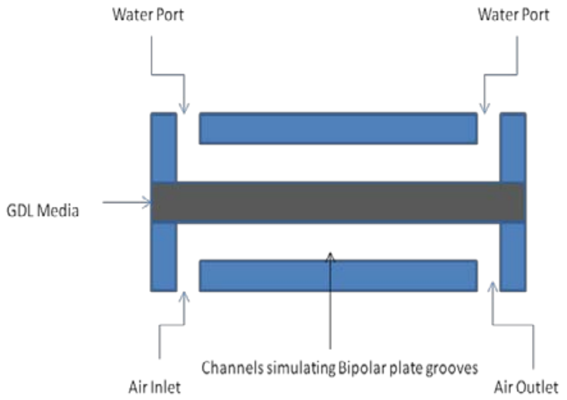
Water and GDL above Air Channel (Drops, Slugs)



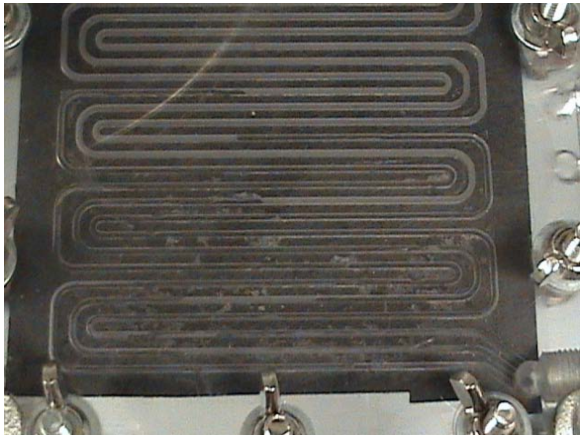
Water and GDL below Air Channel (Film)



- Injecting water through GDL into air channels, evaluating pressure drop and water accumulation versus air flow rate, orientation

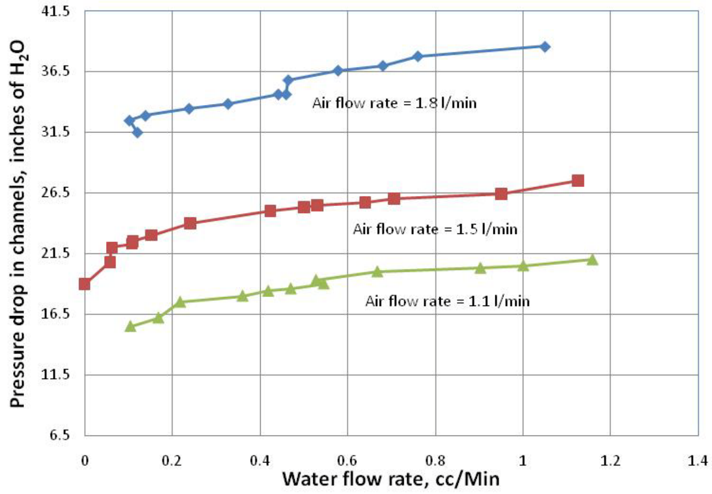


Water accumulation near exit



Serpentine Wet dP: Vertical

Air Outlet at Top (Film)



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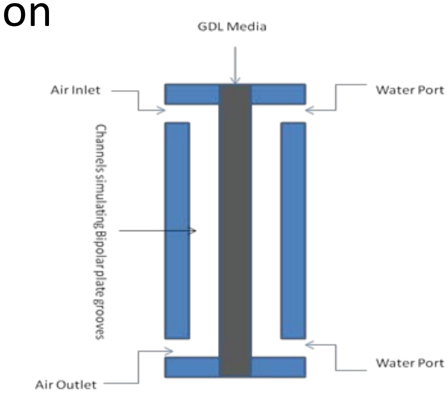
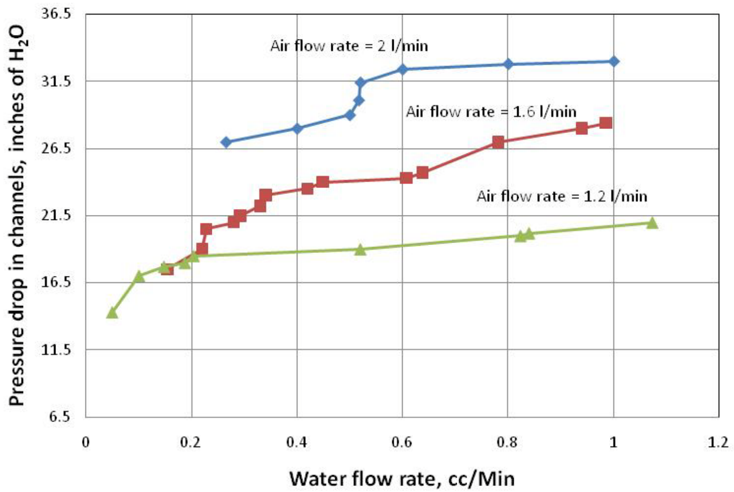
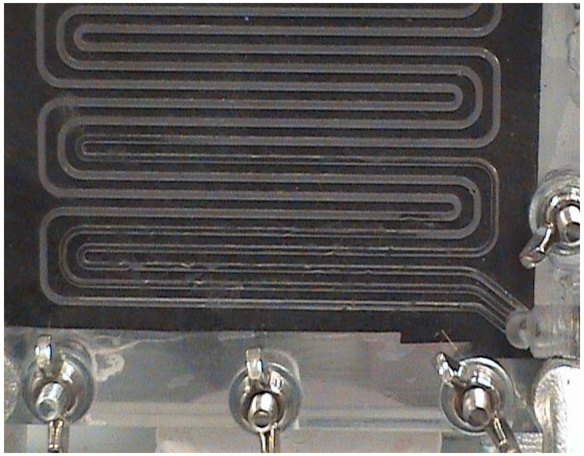


Air Outlet at Bottom (Slugs, Films at high flows)

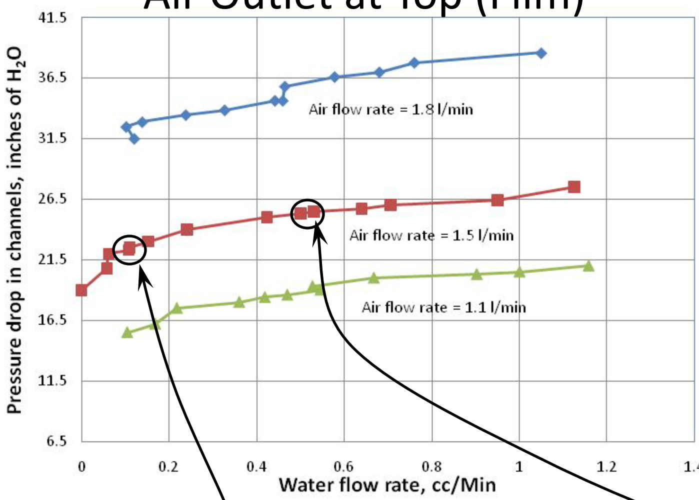


Simultaneous film flow and slugs

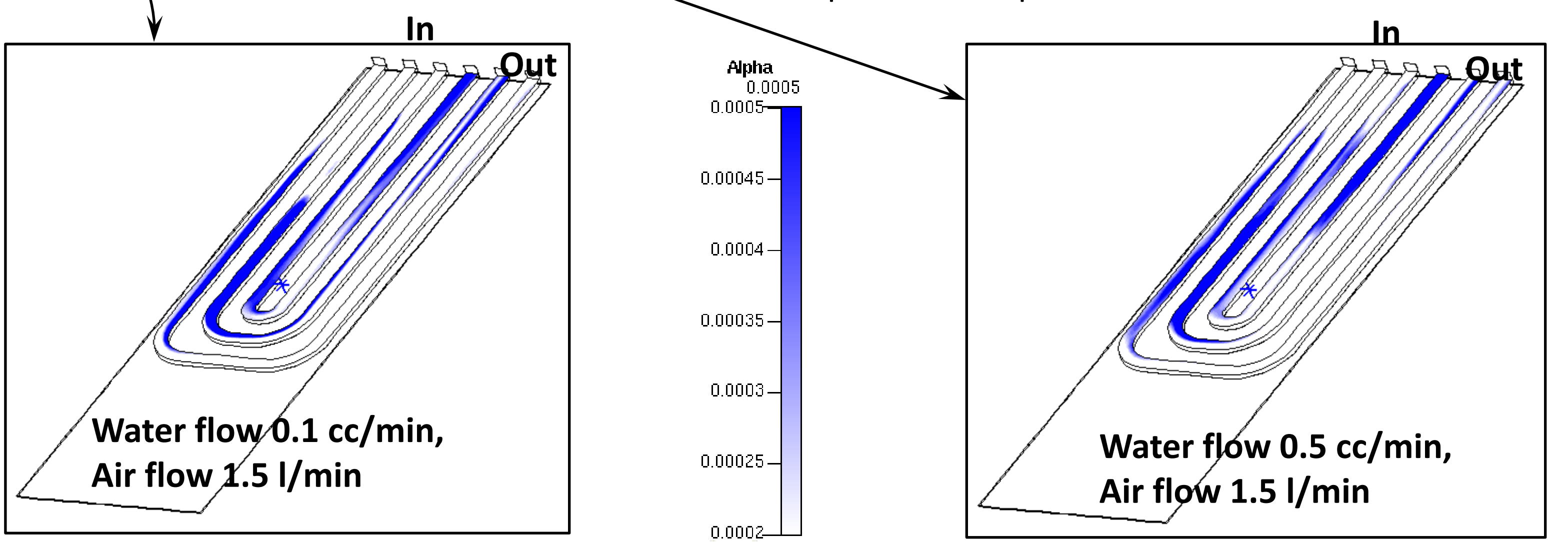


Serpentine Wet dP: Model Test

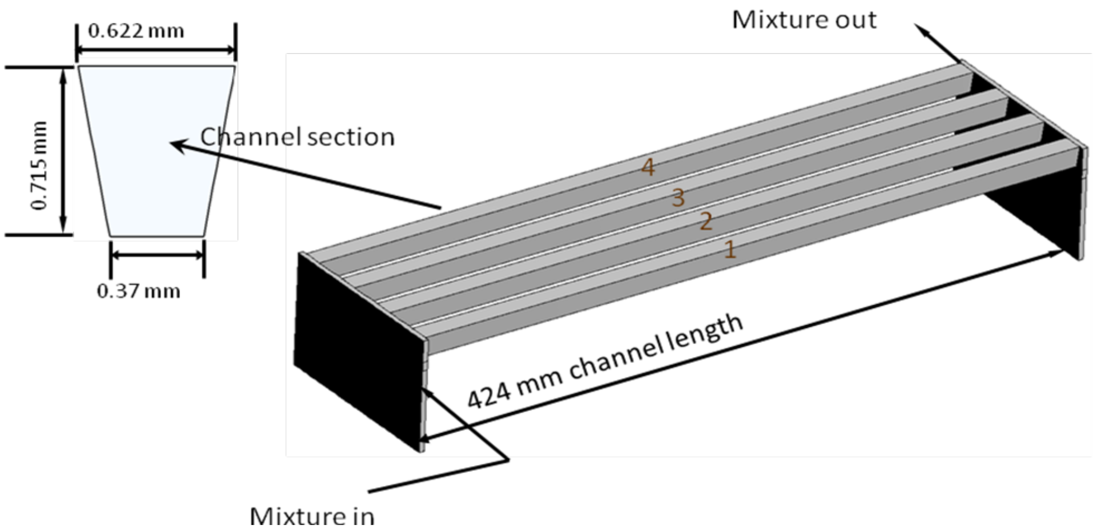
Air Outlet at Top (Film)

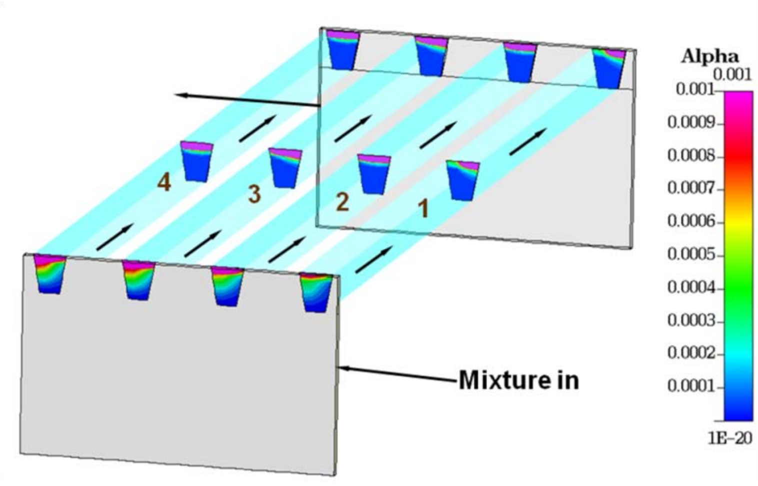


- Testing water permeation through GDL and two-phase pressure drop in channels against experiment:
  - GDL internal contact angle is 120 ° and permeability 1E-11 m^2. The effect of gravity is not included.
  - Pressure drop in the middle channel increases from 2.2 to 2.5 inches of water as liquid flow rate is increased.
  - Extrapolated dP/dL corresponds to 2.7“ H_2O pressure drop difference



Wet Flow Distribution

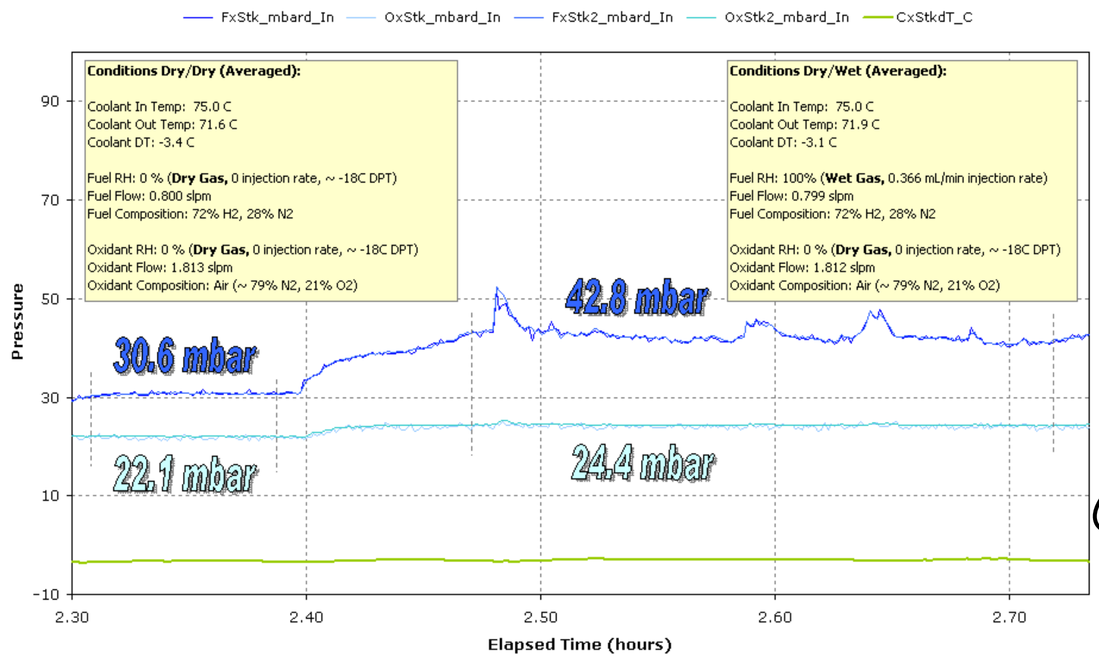


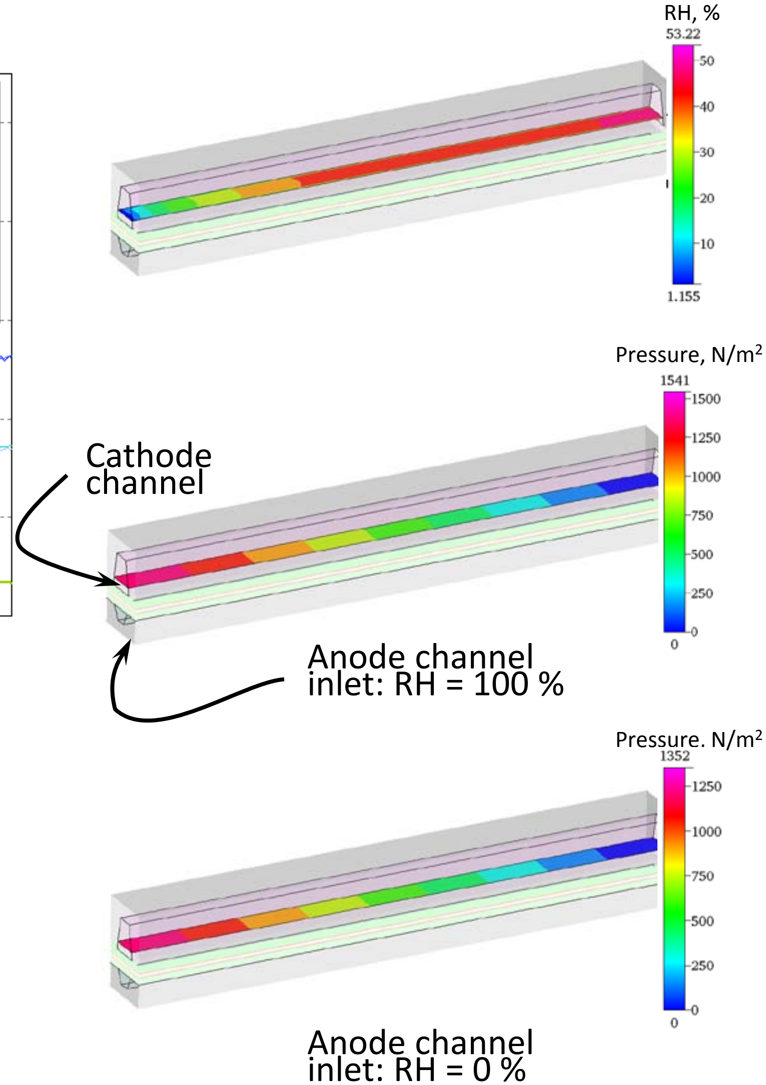


- **Qualitative test of trends for Ballard Baseline channel design:**
  - **Two-phase mixture introduction at side of inlet 'manifold', fixed phase velocities and liquid fraction**
  - **Water preferentially enters channel 4, farthest from inlet, due to greater momentum**
  - **Despite low volume fraction, as liquid water fraction increases, pressure drop increases and air flow rate decreases**

Channel	Air Mass Flow Rate, kg/sec	Water Mass Flow Rate, kg/sec	Pressure drop (Pa)
1	1.10E-05	1.04E-06	17549
2	1.08E-05	1.89E-06	17580
3	1.07E-05	2.53E-06	17583
4	1.06E-05	3.05E-06	17597

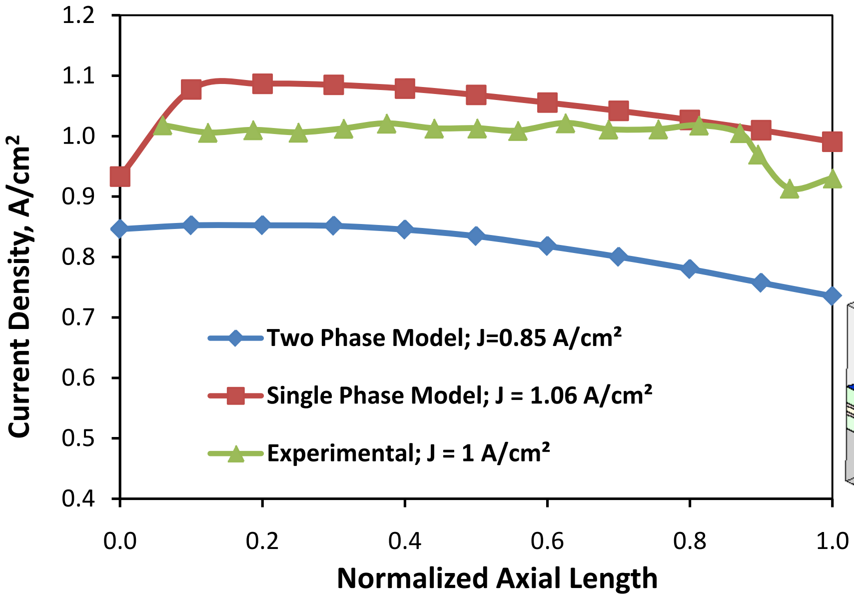
Membrane Water Transport Model Evaluation

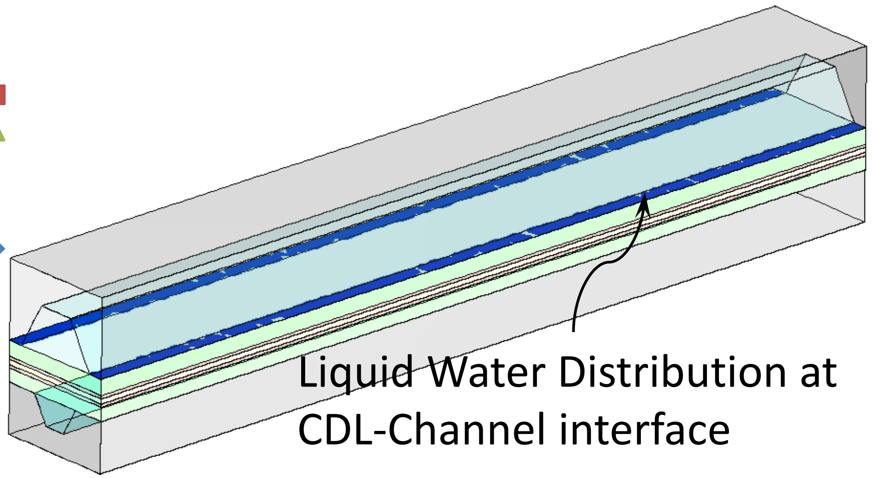




- Ballard observed a 10% increase in the dry air pressure drop as fuel was switched from dry to 100%RH without changing the cathode inlet conditions, suggesting significant water cross-over even in non-operational cell.
- Simulations of water transport, including the Springer membrane water content diffusion model, predicted a 14% increase in pressure drop through the cathode channel

Model Evaluation for Operational Cell

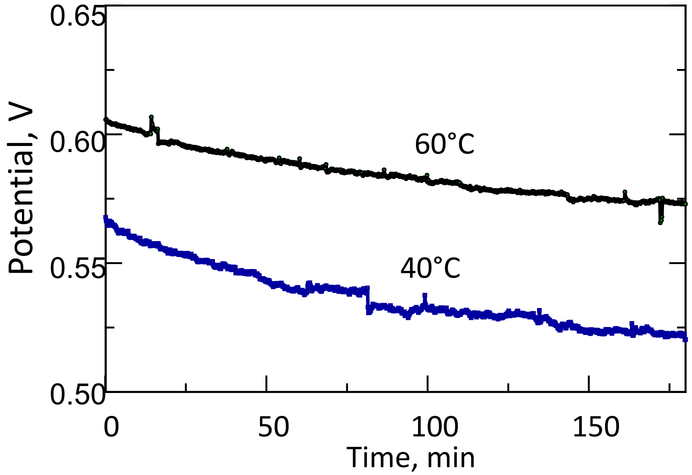


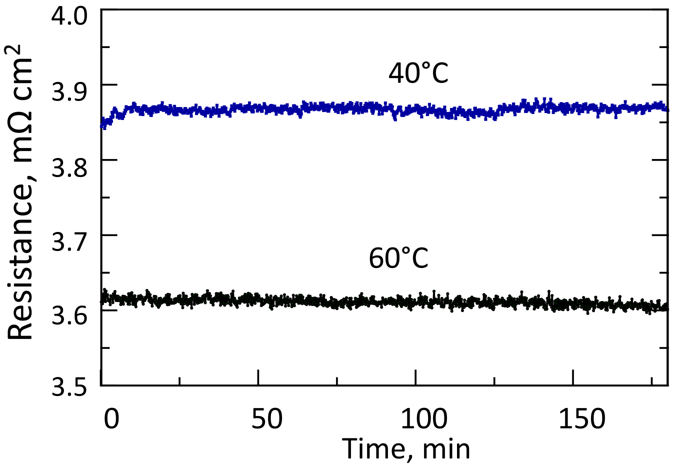


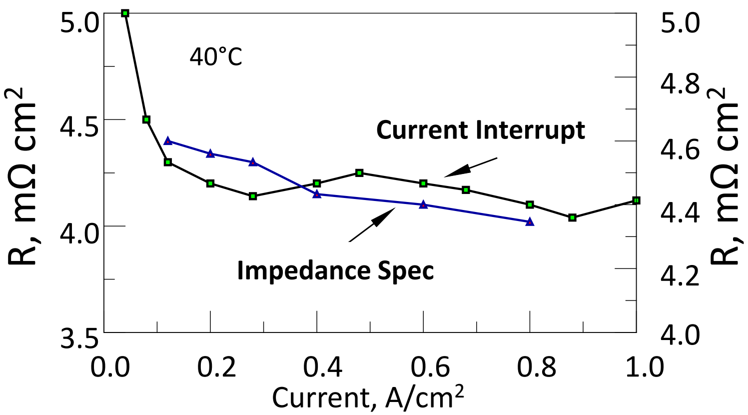
- Integrated two-phase flow, electrochemistry, and heat transfer with ORR forming vapor or liquid phase water based on local thermodynamic state
- Operating conditions: RH Cathode 84%, Anode 41%; Tox 66 °C, Tfuel 74 °C; P=3 atm; Cathode stoich 1.66, Anode stoich 1.5*
- Preliminary results demonstrate improved agreement with current density distribution, particularly at inlet
- Improved treatment of water evaporation/condensation and coupling with membrane hydration identified as routes for further improvement and validation

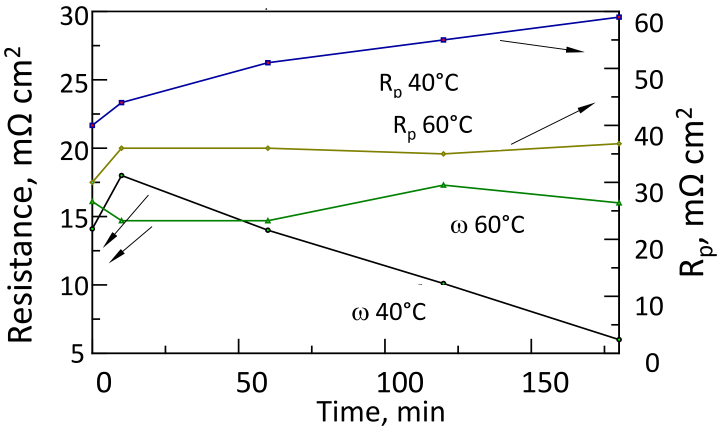
* Ref P.C. Sui, S. Kumar, N. Djilali, *J. Power Sources*, 180, pp. 410–422 (2008) and pp. 423-432 (2008)

IS and CI MEA Hydration Diagnostics





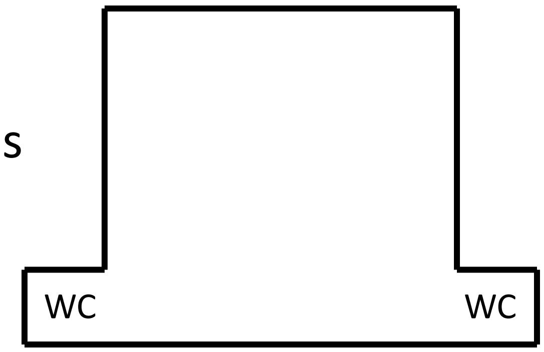




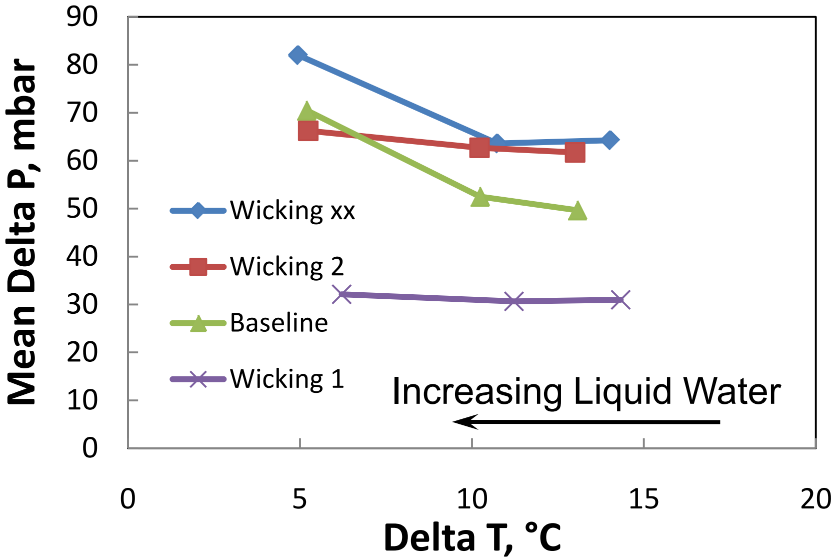
- BCS used low Teflon®, flooding-susceptible GDLs and Impedance Spectroscopy to support conclusions drawn from previous results based on cell performance and Current Interruption measurement.
- High-frequency loop (activation) characteristic frequency and polarization resistance correlated with flooding
- Continuing to optimize water management in MEA, identified intermediate PTFE loading as optimal for a particular GDL to best balance mass transport and water retention near ionomer.

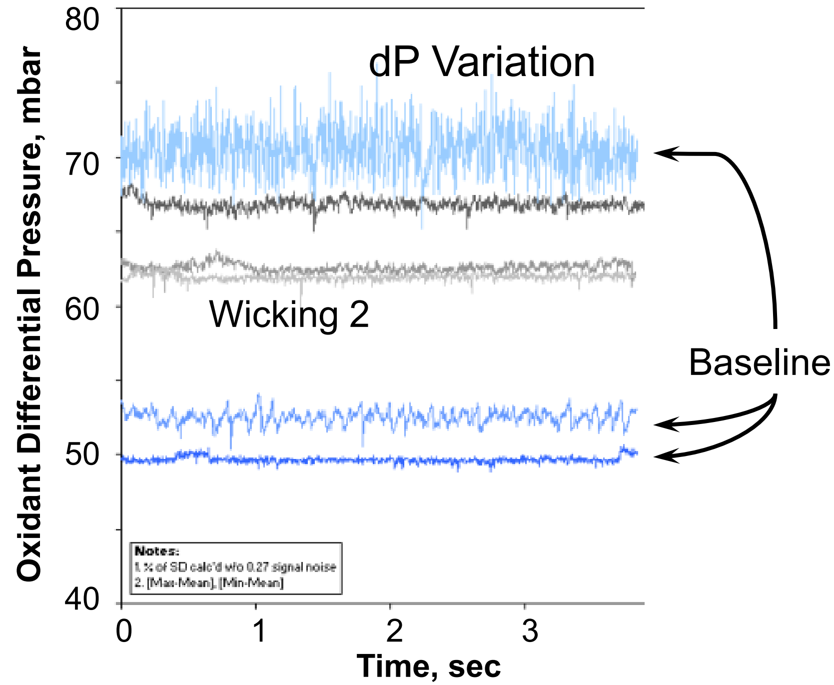
Channel Design for Water Management

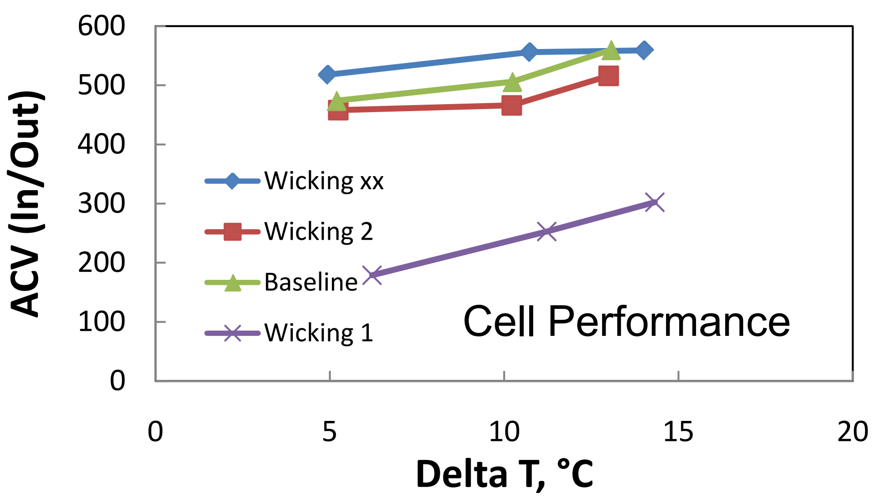
- Ballard and others have identified Wicking Channel Designs as promising candidates for water management. An optimization between the size of the wicking channels and the size of the main channel is important to ensure they manage water in an optimum manner
- Cell performance, which is a function of mass transport and contact area resistance, can be optimized to obtain good performance in wicking designs
- Further improvement in water management is possible by hydrophilic surface coatings for channels and can also be applied to wicking channel designs for additional gains



Initial Screening of Channel Concepts







- Initial studies demonstrate ability to improve pressure drop and pressure variation over a range of operating conditions (liquid water)
- Cell level optimization still required to improve performance over a broad range of operating conditions

Interactions/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

Future Work and Milestones

FY10-11 Plans:

- Model Development/Testing
  - Improve integration of heat transfer, particularly evaporation and condensation, and membrane water transport with two-phase CFD models (CFDRC, ESI)
  - Continued improvement of numerical stability and prediction of operational cell data (CFDRC, ESI)
  - Cell-scale model evaluation against steady and transient data (CFDRC, Ballard)
- Water Management Improvement
  - Experimental and Simulation Parametric Studies Focusing on:
    - Materials modification, primarily GDL selection and treatment, and operating strategies (BCS, Techverse, CFDRC)
    - Channel design, surface finish, and GDL design for effective removal with low pressure drop (Ballard, CFDRC)

Upcoming Milestones:

- Final model improvements and code package development complete March 2011
- Assemble, test, and demonstrate improved self-humidified cell June 2011

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:
  - Generated flow regime map from droplet emergence at GDL-channel interface studies; demonstrated improved model agreement with transition from film flow to droplet regime
  - Implemented experimental setup for collecting wet pressure drop and transient pressure signatures in two-phase flows in channels and cells; improved agreement of model predictions and observed wet pressure drop
  - Integrated electrochemistry, heat transfer, and phase change with the CFD two-phase flow models and demonstrated improvement in current density distribution for initial validation test case
  - Identified materials and design modifications to focus on for improved water management
- Proposed Future Work:
  - Improve 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 the identified optimization strategies: Channel design, surface finish, and GDL design for effective removal with low pressure drop; GDL design and treatment for improved cell performance