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

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Overview

- **Timeline**
  - **Start Date: 6/1/07**
  - **End Date: 11/30/11**
  - **Percent Complete: 85%**
- **Budget:**
  - **Total Project Funding:**
    - **DOE $4,958K**
    - **Contractors $1,463K**
  - **Funding Received in FY10**
    - **$1,175K DOE**
    - **$295K Cost Sharing by Team**
  - **Funding for FY11**
    - **$818 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

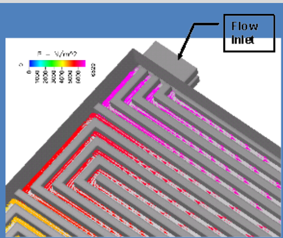
- **Overall:**
  - **Improve understanding of the effect of various cell component properties and structure on the gas and water transport in a PEM fuel cell;**
  - **Demonstrate improvements in water management in cells and short stacks; and**
  - **Encapsulate the developed understanding in models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

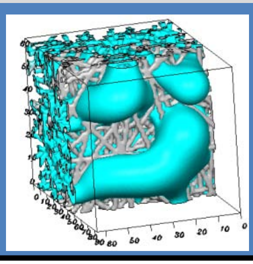
- **FY 2010 and 2011:**
  - **Evaluate cell-scale water transport models on component and operational cell level; validate and apply to sensitivity studies**
    - **Data and tools for screening of concepts to improve water management while increasing power densities, mitigating liquid-water induced pressure drops and transients for system-level benefits**
  - **Develop and evaluate concepts for water management improvement**
    - **Component interaction and flooding sensitivity studies for performance improvement**
    - **Channel design and GDL modification for effective water removal with low pressure drop**

Approach

Improved Water Management Through Improved Component Designs and Operating Strategies

Advanced Model Development (CFD/LBM)

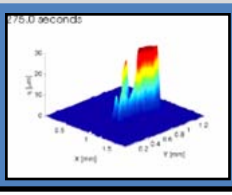


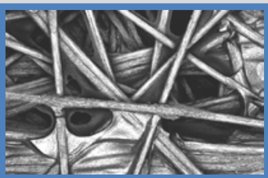


- **LBM models for microscale flow thorough porous media: in-plane and through-plane permeabilities, capillary pressure, and wetting characteristics**
- **CFD models for macroscopic two-phase flow in channels, GDLs and interfaces, coupled with electrochemical reaction and transport through membrane**

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

Experimental Characterization



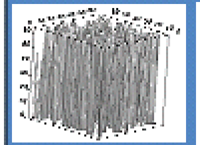


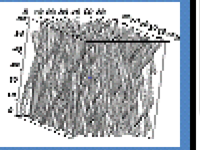
- **Ex-situ characterization: key materials properties and sensitivity to treatments, water transport analysis in GDLs and micro-channels**
- **In-situ diagnostics: current and water distribution**

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	
400 µm/16 mil		GDL 10	3 D - nonwoven





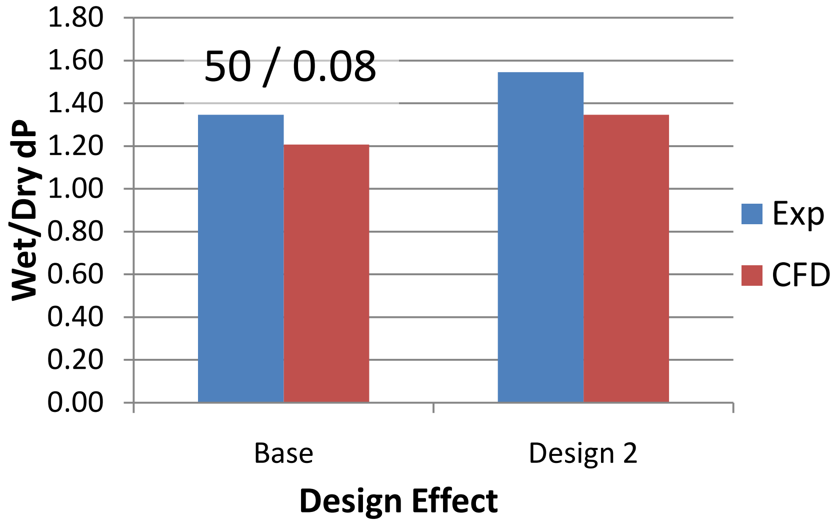
- **Cell flooding sensitivity to materials and operating strategies**
- **Implement and test performance improvement strategies**

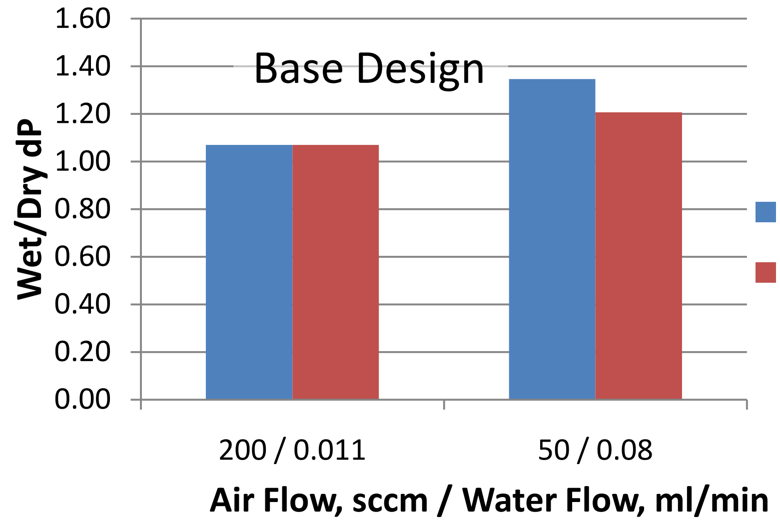
Improved component designs and operating strategies, tools for addressing water transport in future generation designs

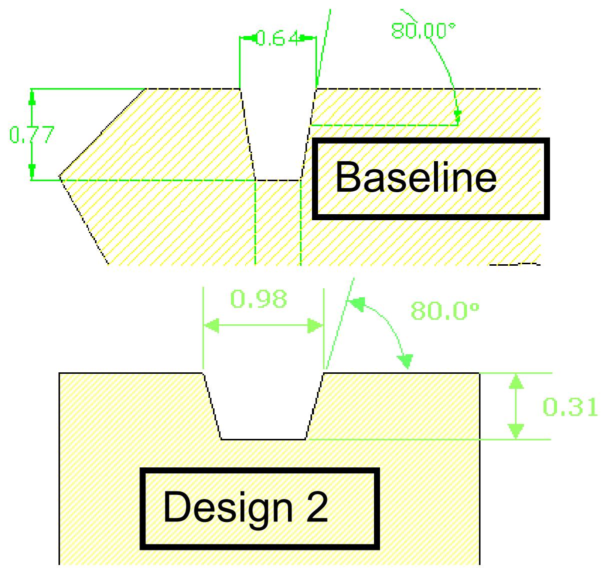
FY 10-11 Plans and Milestones

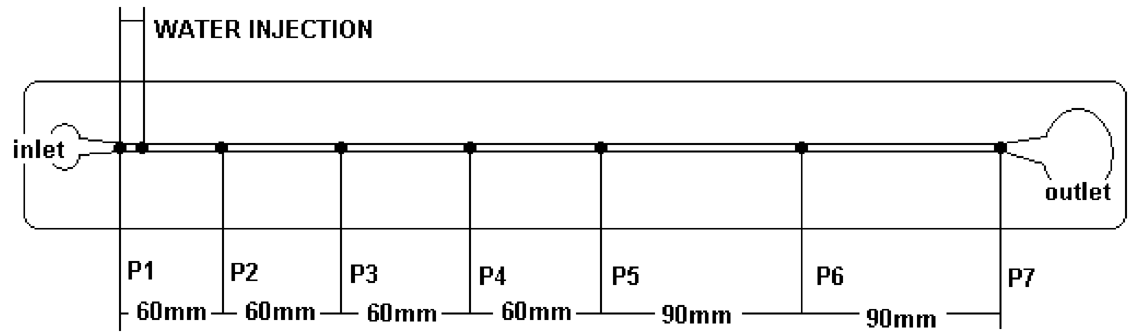
Month/Year	Milestone	Comments	% Complete
Mar 11	Cell scale models tested and validated against steady and transient operational cell data	Progressing for steady state; transients needed to address extreme conditions	75%
Mar 11	Complete fuel cell water transport model improvements and code package development	Revised to 9/31/11, Includes testing against experimental data gathered during 3/11-9/11	50%
May 11	Complete validation of water transport model and make recommendations for water management improvement	Revised to 10/31/11	50%

Model Evaluation: Two-Phase Channel dP with GDLs





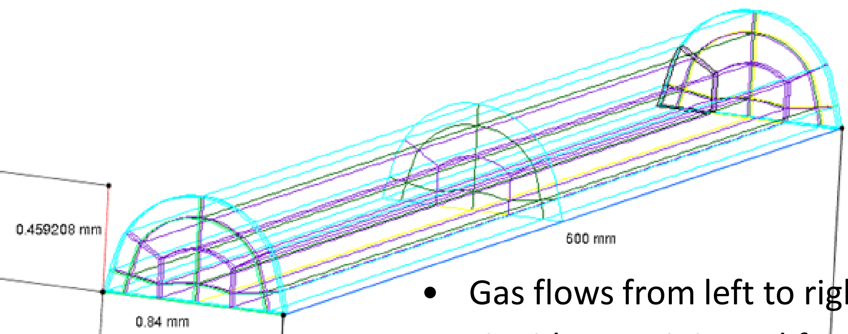




- Ballard Two-Phase dP measurements, injecting water through GDL at channel top
- Models capture trends with design variation and operating conditions

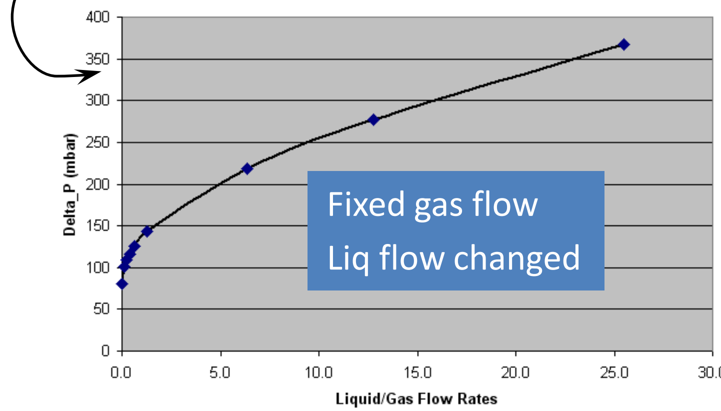
Liquid Water Impact on Pressure Drop

Ballard Design Cathode Channel



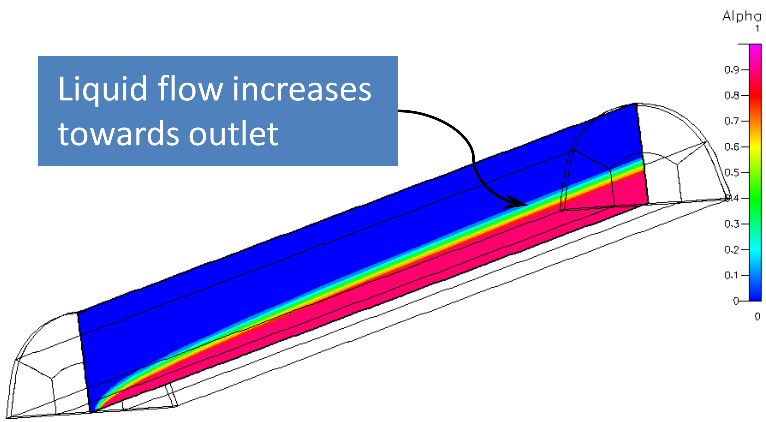
- Gas flows from left to right
- Liquid water injected from bottom channel wall to evaluate effects in model

Experimental ~ 340 mbar @ 1A/cm2

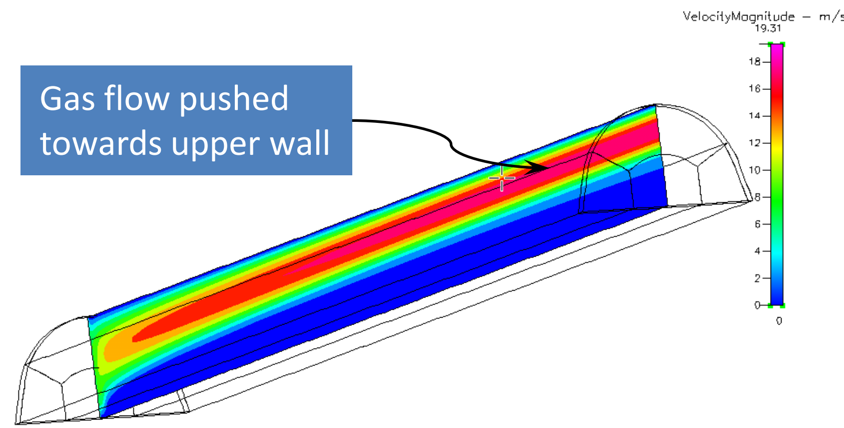


Increasing DP predicted with Liquid Water

Liquid flow increases towards outlet



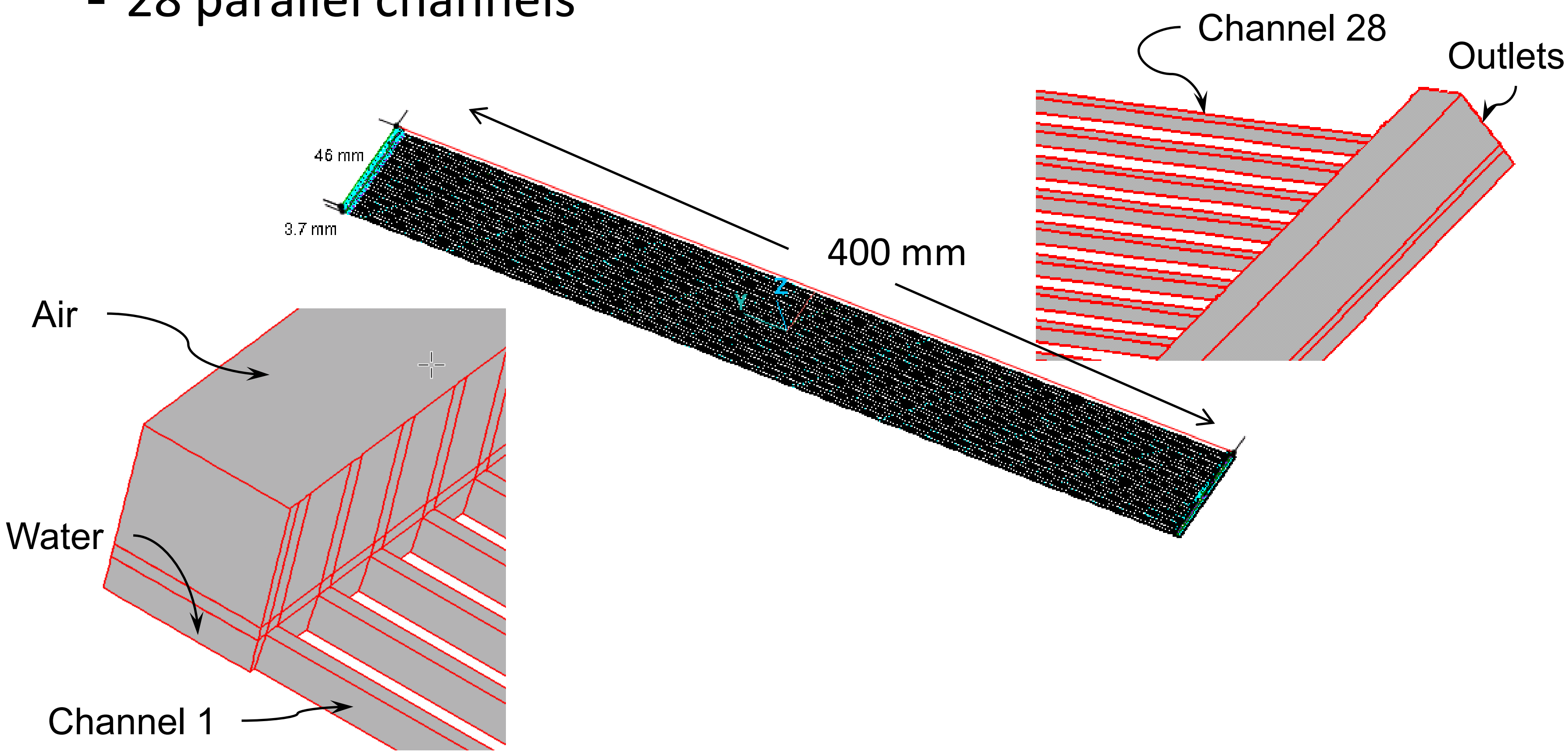
Gas flow pushed towards upper wall



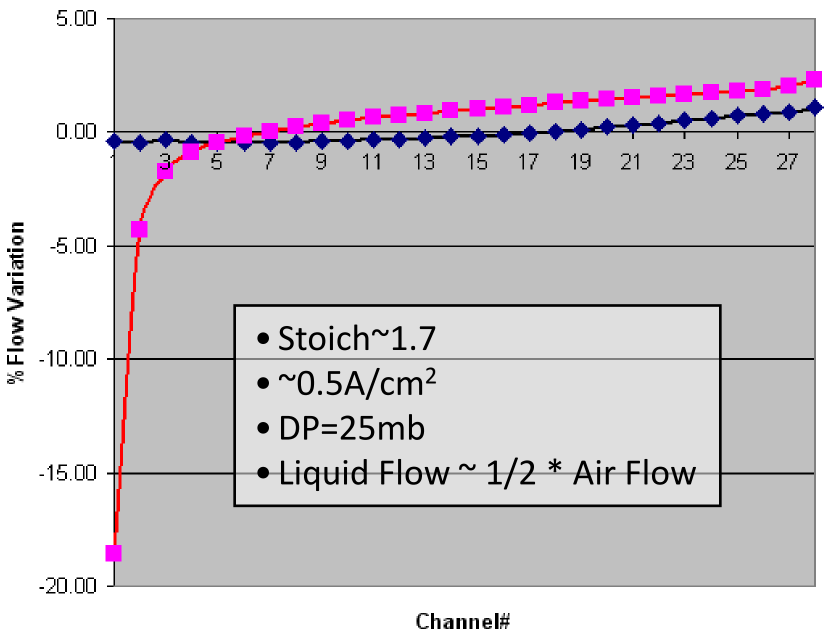
- Ballard study of forward prediction of wet pressure drop, indicating extent of channel water corresponding to observed operational pressure drops

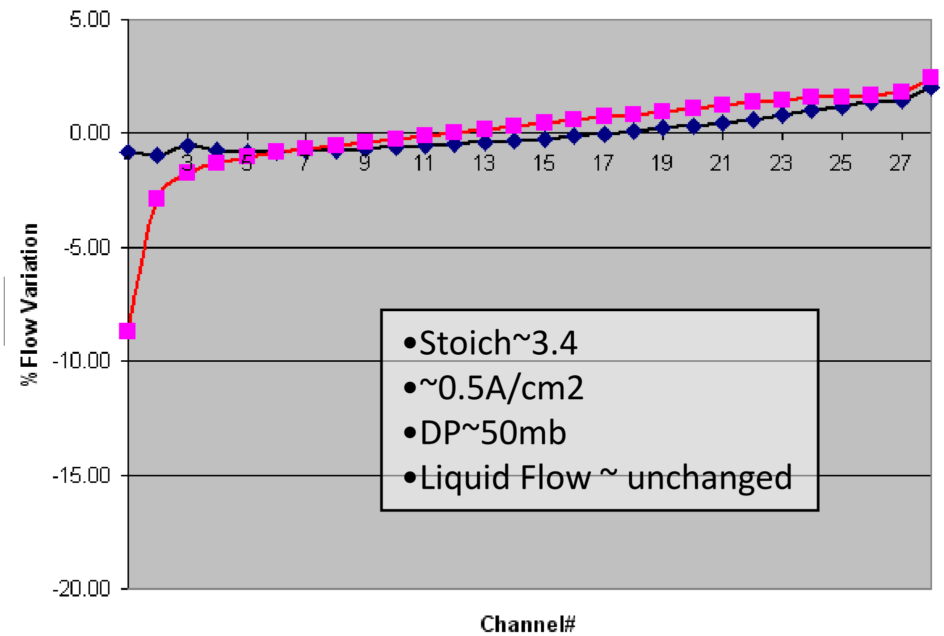
Channel/Channel Flow Sharing Analysis

- Ballard study for a low pressure drop cell design
- 28 parallel channels



Liquid Water Impact on Channel/Channel Flow Sharing

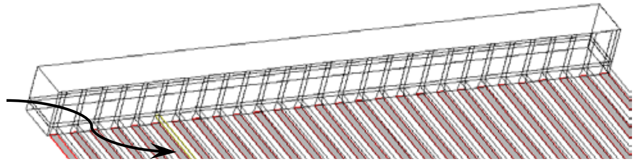




- Wet Flow Sharing is 20.9% compared to dry case at 1.6% under initial (left) scenario
  - Most of the liquid water enters first few channels, the first channel being the worst with nearly 18.6% below the average flow
- Doubling air flow (right): Wet Flow Sharing is 11.2%
  - First channel air stoich improved from 18.6% to 8.7% below average as air stoich increased
- Models allowing forward prediction of liquid water impact in Cells and Channels

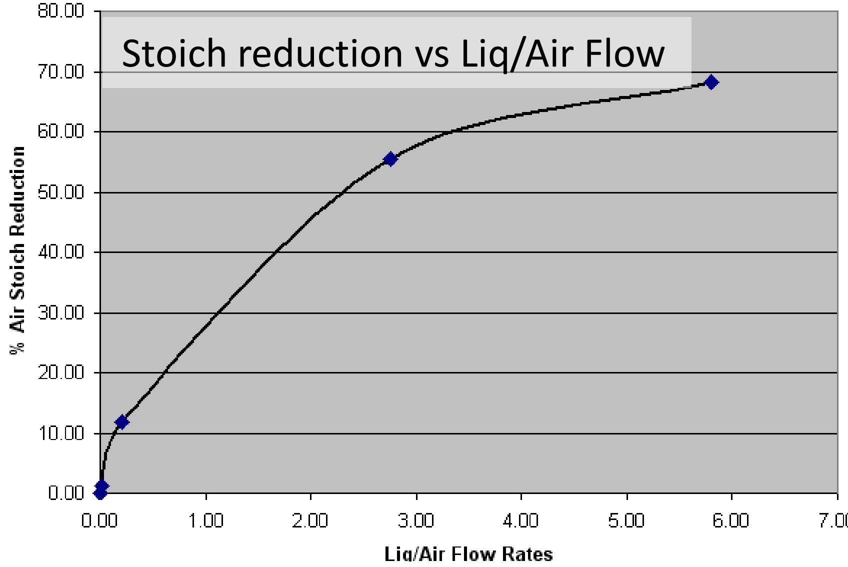
Liquid Water Management in Cells

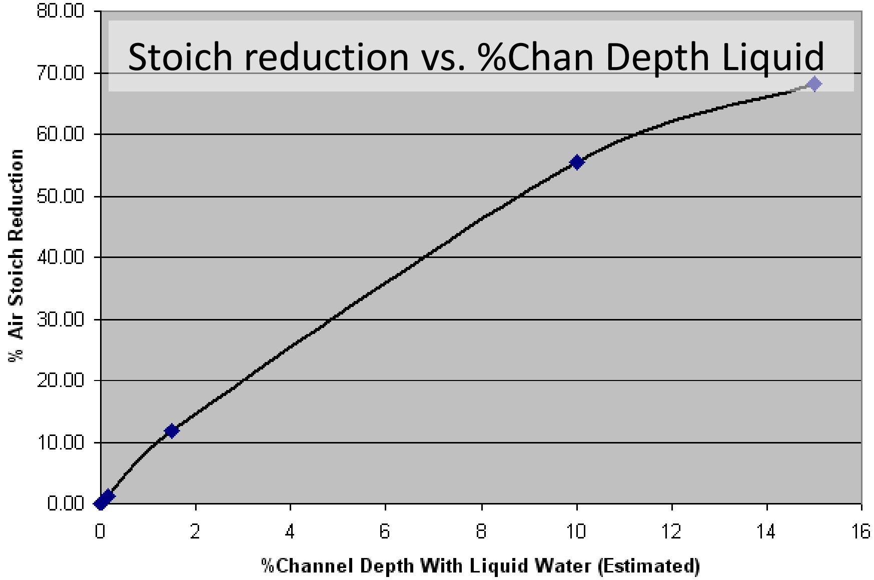
- Ballard study of Low DP baseline cell with 28-channels is modeled at 25mbar fixed Cell dP to simulate the "cell in stack behavior" for predicting how poor channel water management (i.e. more channel water) causes air stoich reduction which will lead to cell mal-performance.
- All channels in the cell have equal liquid water flux from "wall" corresponding to GDL surface



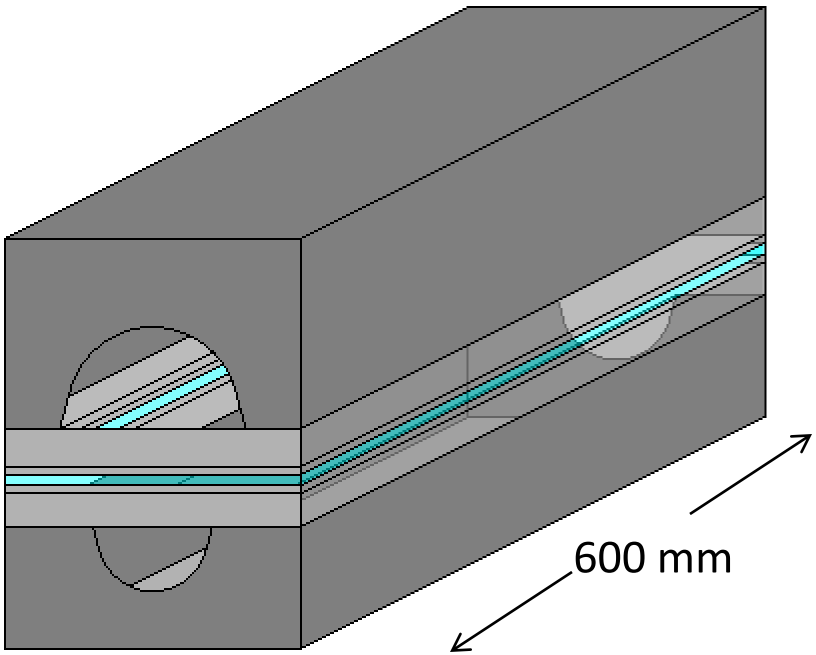
- Liq/Air Flow = 0.02 is when all the water produced at 1 A/cm^2 will remain in channels of the cell and represents 0.15% channel depth for liquid blockage

Two Fluid Model used to forward predict the impact of liquid water on cell stoich reduction

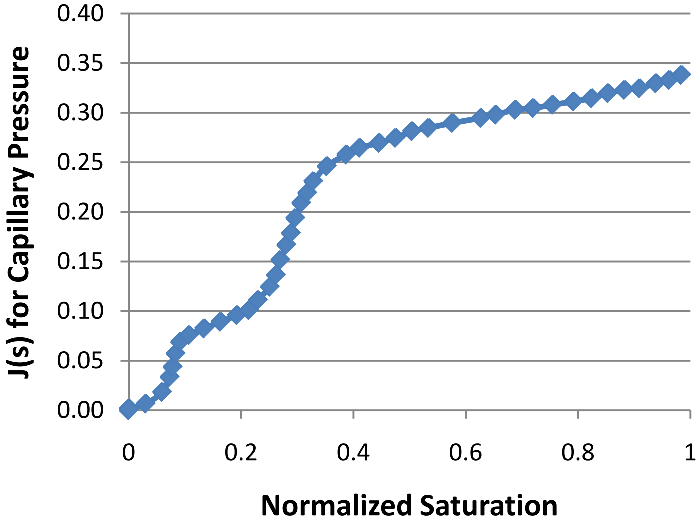




Ballard Design Cell Model

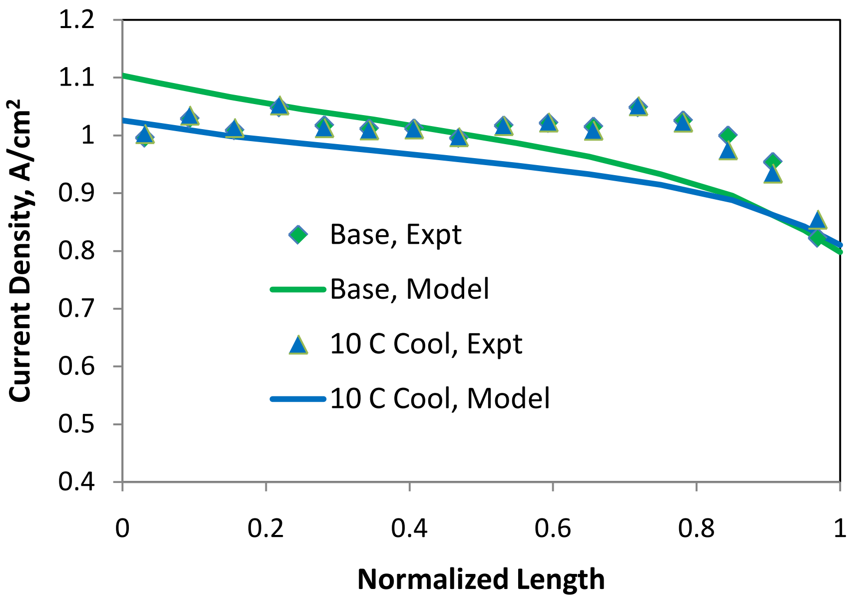


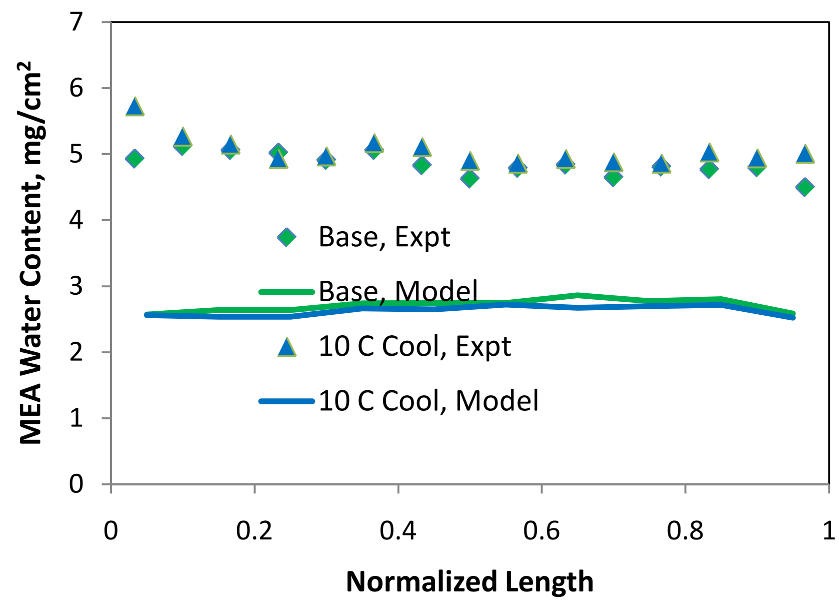
Saturation dependence of capillary pressure used in the models, residual saturation 0.2



- Layout of operating cell model: counterflow cathode and anode, symmetry conditions to reflect multiple channels in parallel
- Cooling channel effects approximated with linear applied temperature profile based on measured/controlled values
- Full two-phase flow model in channels and porous regions coupled with heat and mass transfer, electrochemistry, and Springer model for membrane water content

Operational Cell Model Evaluation

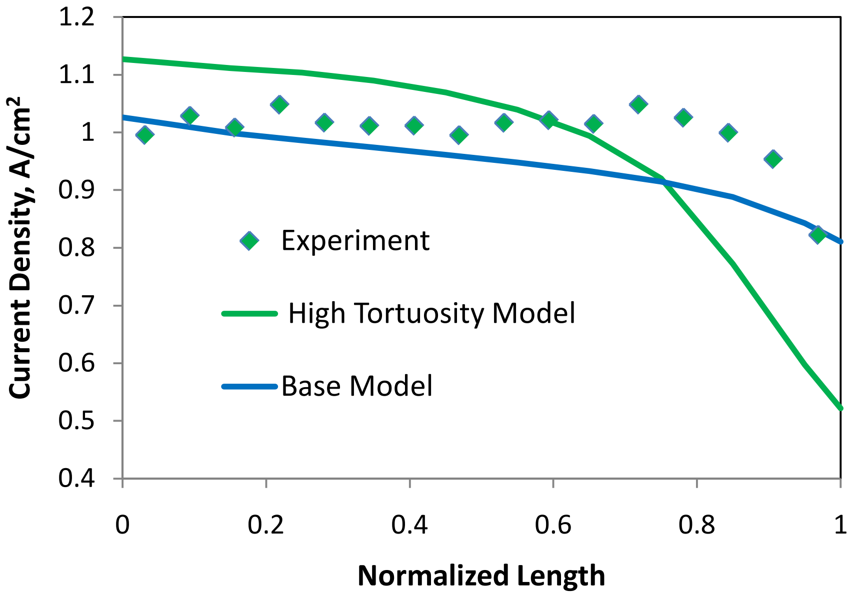


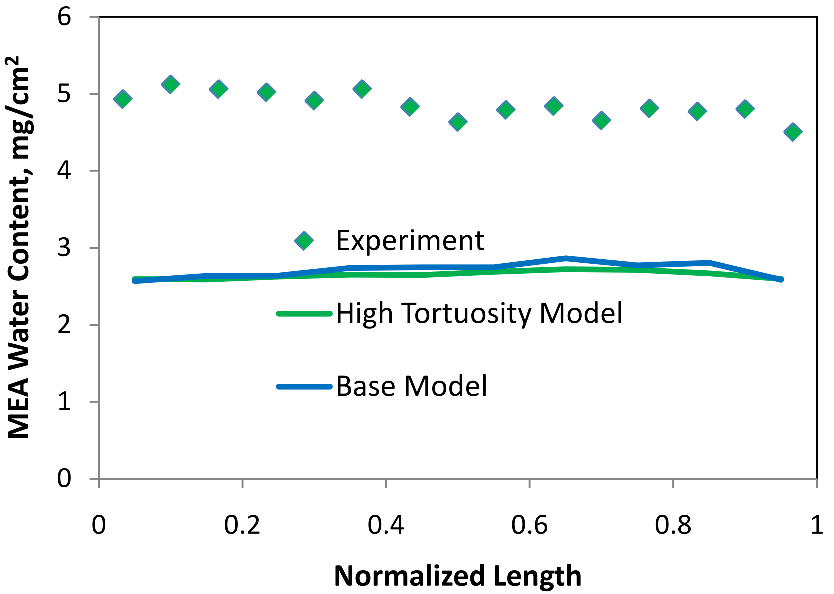


- Base conditions 1 A/cm^2, Ox 87% RH stoich 1.8 at 3 bar, Fuel 46% RH stoich 1.6 at 3.2 bar, coolant 65°C in 75 °C out
- Model operated at fixed bias corresponding to measured voltage, parameters from Sui et al* and Ballard
- Water content under predicted in both membrane and GDL

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

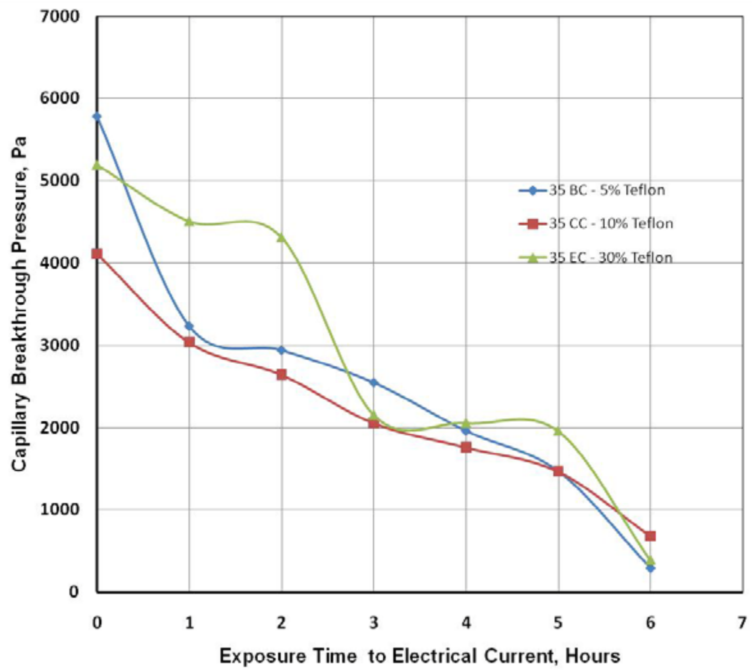
Operational Cell Model Sensitivity

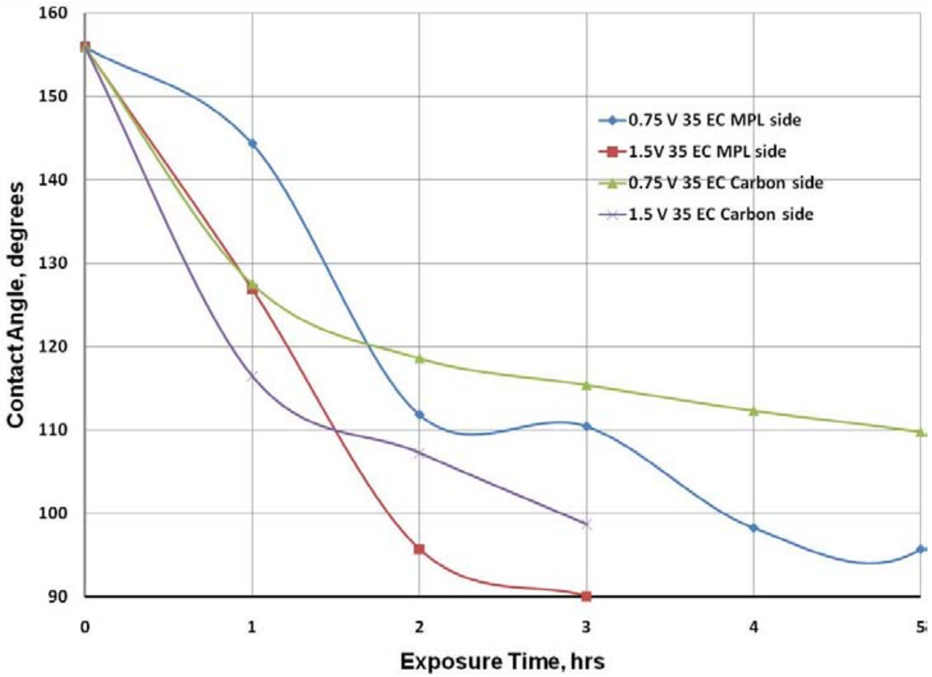




- Modified GDL properties to match measured data:
  - Increased model GDL tortuosity to 4 from 1 to match measured through-plane effective diffusivities
  - Increased through-plane GDL permeability from 1 Darcy to 3 Darcy, in-plane to 12 based on measured values
- Increased membrane equilibrium water content at saturation to 22
- Model is oxygen transport limited near cathode exit

GDL Materials Evaluation: Accelerated Aging



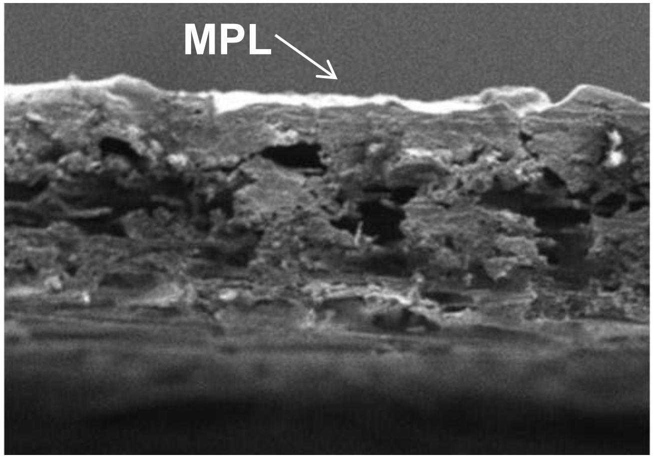


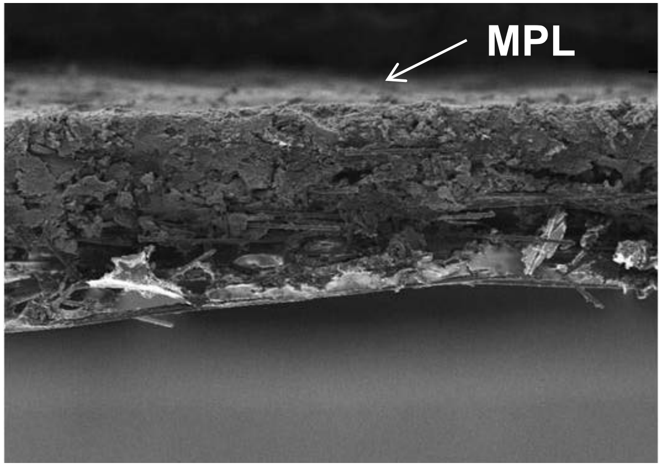
- Techverse performed aging studies ex-situ by applying bias to humidified GDLs:
  - Focused on determination of the change in the properties of GDL media when exposed to electrical current as would be the case in a working PEM fuel cell
  - Commercial media found to lose hydrophobicity as evidenced by reduced capillary breakthrough pressure and surface contact angle; increased water permeability
  - Increased current level accelerated the rate of loss of hydrophobicity as determined by surface contact angle

Images of Teflonated GDL Media Response

Before | **After**

Cross Section



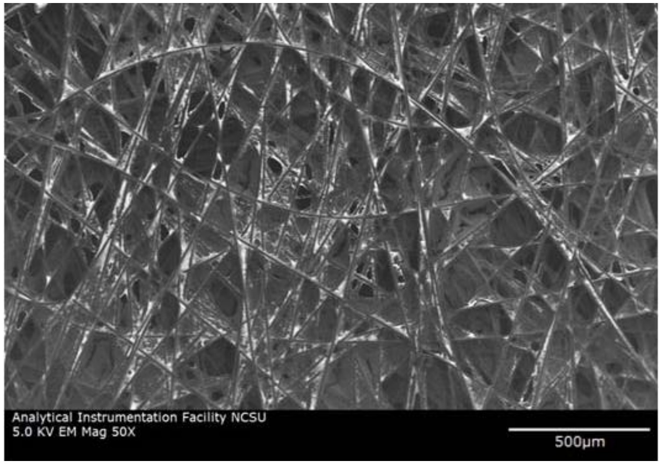


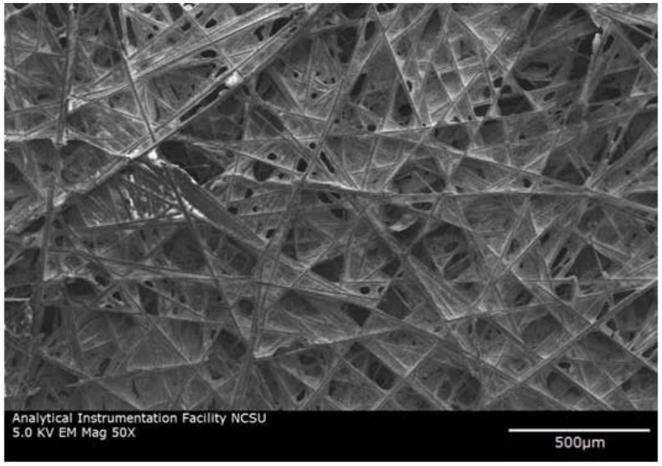
- ve electrode

e^-

+ ve electrode

Surface on Lower edge

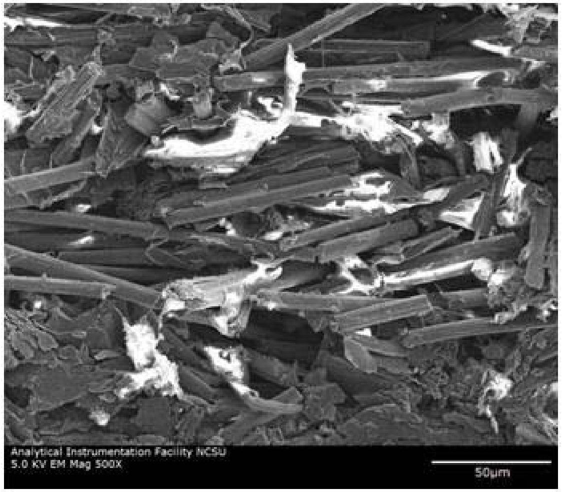


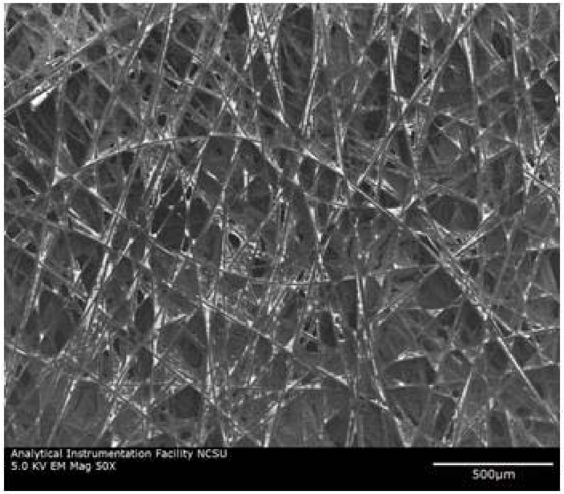


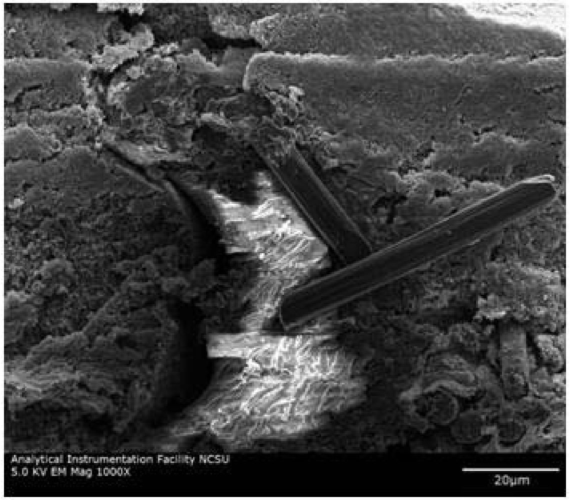
- SEM of SGL Carbon 35 EC media, approximately 30% PTFE loading

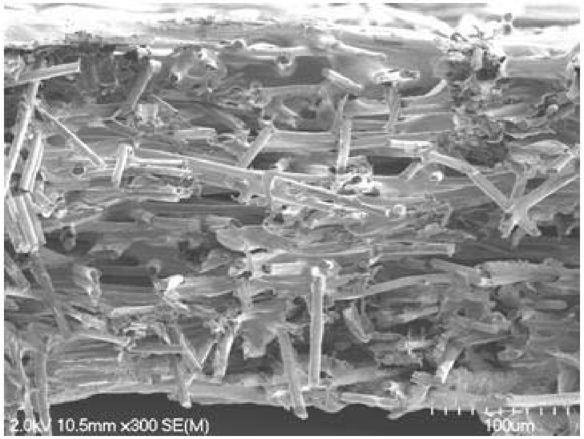
Teflon® Fiber Coverage Comparison

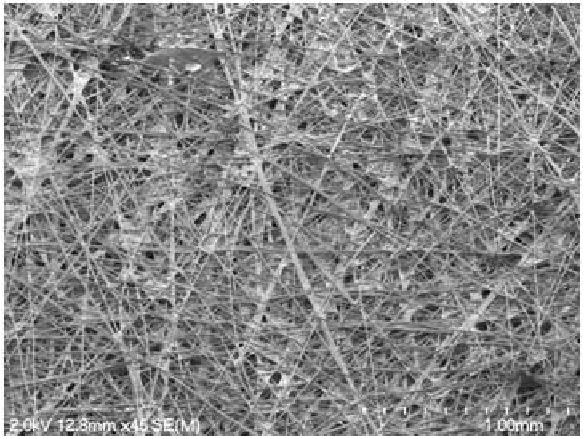
SGL Carbon 35 EC media – carbon paper with 30% Teflon®









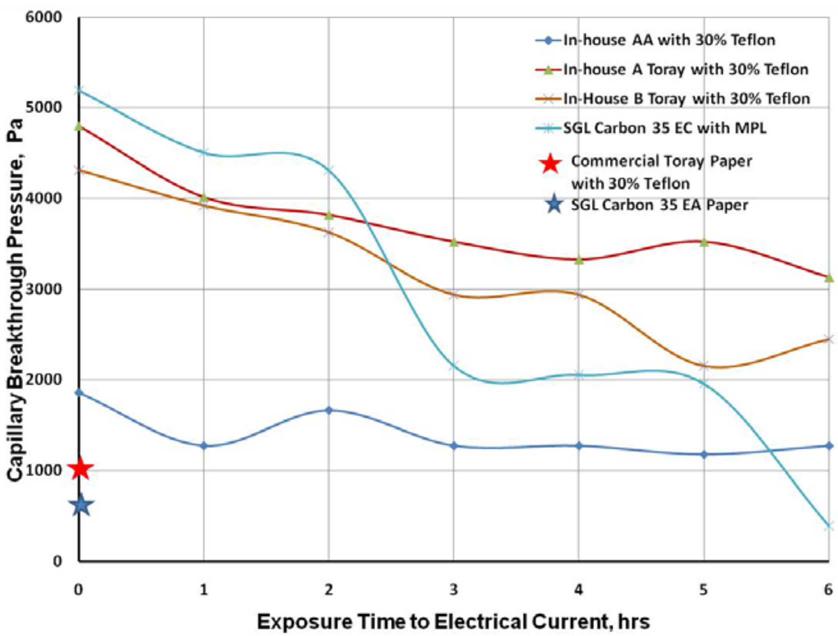


Electrophoresis treated SGL 35 AA media - 30% Teflon®

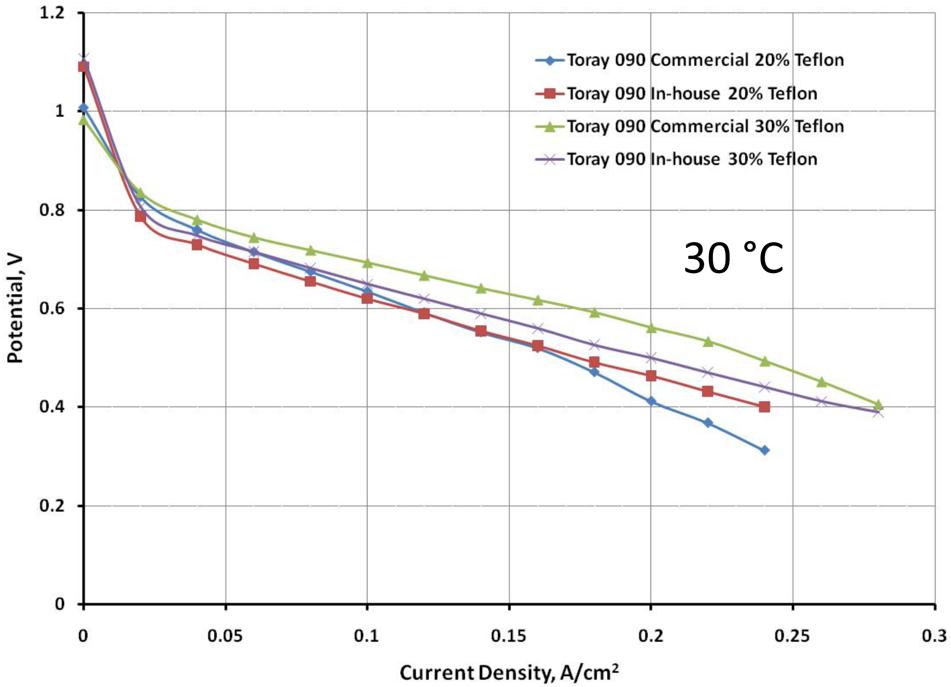
Comparison of GDL Properties

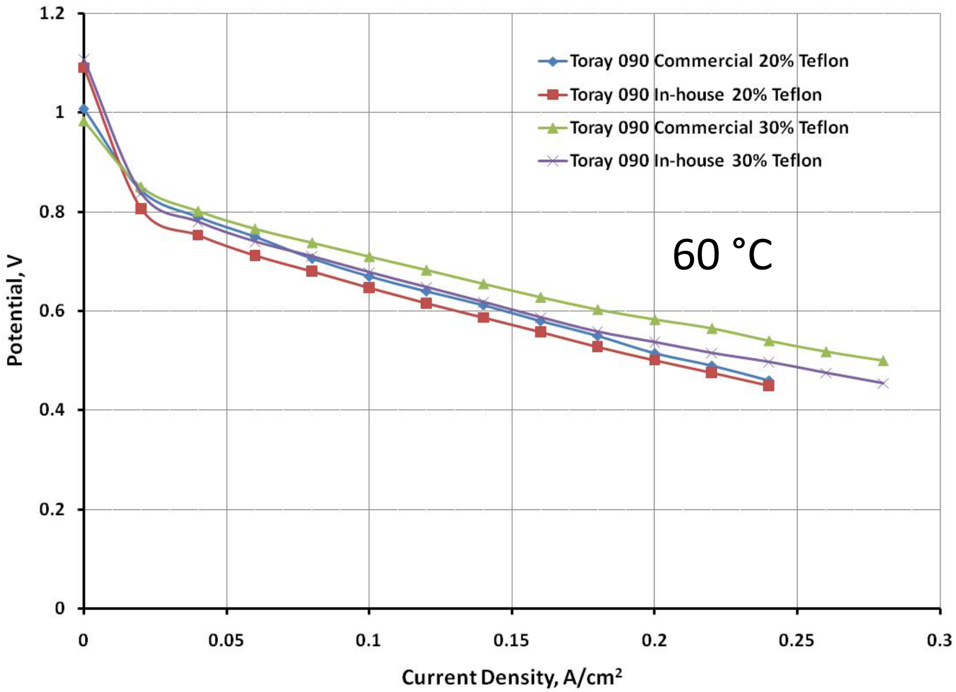
- Developed coating of carbon fibers by electrophoresis, in contrast to commercial media, leads to:
  - More uniform PTFE coatings for lower residual saturation, increased hydrophobicity at equivalent loadings
  - Better retention of hydrophobic properties in simulated aging experiments

Sample	Residual Saturation	Breakthrough Pressure
n/a	%	Pa
35 EA - 30% Teflon	15.52	587
35 DA - 20% Teflon	25.54	1077
35 CA - 10% Teflon	7.6	1175
30% in-house AA sample	2.44	1959
7.5% in-house AA sample	2.32	1763
30% in-house A Toray	0.416	4800
15% in-house A Toray	0.6	3400
6% in-house A Toray	0.8	3100
30% in-house B Toray	0.769	3918
18% in-house B Toray	0.9	3300
4% in-house B Toray	1	3100
10% commercial Toray	3.3	780
20% commercial Toray	4	1000
30% commercial Toray	2.5	1100



GDL Comparison: Single-Cell Performance





- Electrophoresis-treated and commercially available media, initial evaluation by BCS Fuel Cells:
  - MPL is needed for good performance in BCS MEAs under standard operation, development of MPL process in progress
  - Electrophoresis impregnated media indicates greater resistivity due to fiber coating
  - Slightly higher open circuit voltages with electrophoresis impregnated media

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
  - Techverse: Materials characterization and modification
  - BCS Fuel Cells: Operational cell and stack diagnostics, materials sensitivity and serpentine channel design
  - ESI Group, NA: Model implementation and software integration, model testing
  - SGL Carbon: GDL and bipolar plate materials
  - U. Victoria: GDL permeation, channel droplet injection and transport quantification

Future Work and Milestones

FY11 Plans:

- Model Testing and Simulation Package Development
  - Cell-scale model evaluation against steady and transient data (CFDRC, Ballard) including current density, MEA water, and crossover; emphasizing extreme conditions for excess water or dryout (temperature, RH, stoich)
  - Continued improvement of numerical stability, user interface and user access to key properties (CFDRC, ESI)
- 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 and operating strategies for effective liquid water removal with low pressure drop (Ballard, CFDRC)

Upcoming Milestones:

- Final model improvements and code package development complete Sept 2011
- Assemble, test, and demonstrate improved self-humidified cell Oct 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:
  - Predicted design and operating condition sensitivity of observed wet pressure drop with experimental measurements of wet pressure drop for two-phase flows in channels and GDLs, began model application to screen channel and cell design
  - Improved stability of two-phase cell scale models, demonstrated improved agreement with measured current density profiles
  - Developed a technique for reproducible, controllable hydrophobic treatment of GDL media
- Proposed Future Work:
  - Refine and validate the developed integrated models using operational cell-scale steady and transient data;
  - Apply validated measurement and simulation tools to assess water management optimization strategies: Channel design for effective removal with low pressure drop; GDL design and treatment for improved cell performance