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

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CFDRC

Prepared for:
DOE Hydrogen Program Annual Review Meeting
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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.**

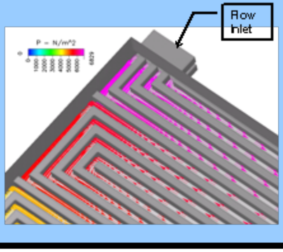
- **FY 2008 and 2009:**
  - **Complete baseline characterization for Gas Diffusion Layer (GDL) materials**
    - **Key fundamental properties affecting water transport**
  - **Gather experimental data under controlled conditions, test and apply models for water transport in GDLs, channels, and across 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**

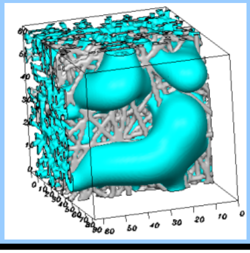
Approach

Experimental Characterization ⟷ Multiphysics Modeling

Improved Water Management Through Improved Component Designs and Operating Strategies

Advanced Model Development (CFD/LBM)

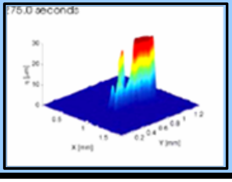


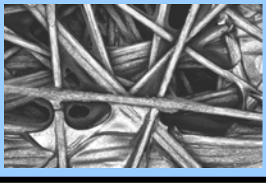


- LBM models for microscale flow thorough porous media: in-plane and through-plane permeabilities, capillary pressure, and wetting characteristics
- CFD models for macroscopic two-phase flow in channels, GDLs and interfaces, coupled with electrochemical reaction and transport through membrane

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

Experimental Characterization

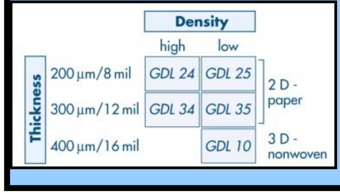




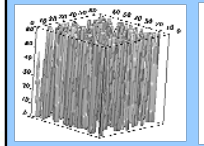
- Ex-situ characterization: key materials properties and sensitivity to treatments, water transport analysis in GDLs and micro-channels
- In-situ diagnostics: current and water distribution

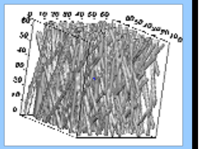
Provides fundamental understanding, validation data for physics-based models from component to cell level

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





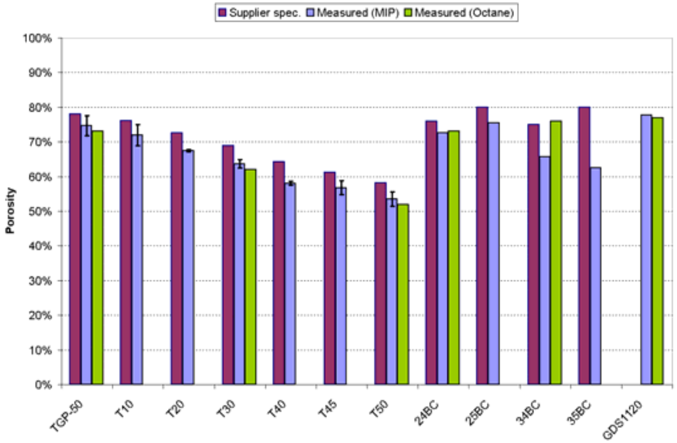
- Cell flooding sensitivity to materials and operating strategies
- Implement and test performance improvement strategies

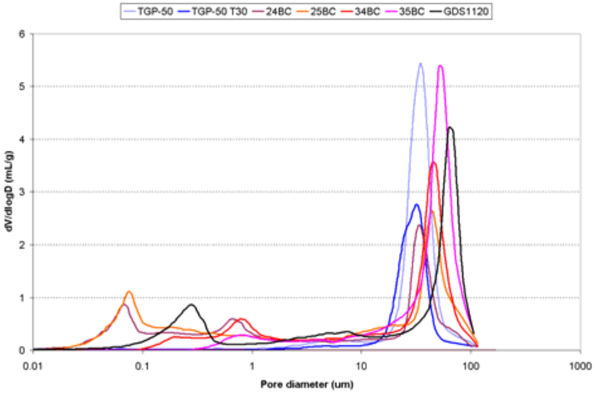
Improved component designs and operating strategies, tools for addressing water transport in future generation designs

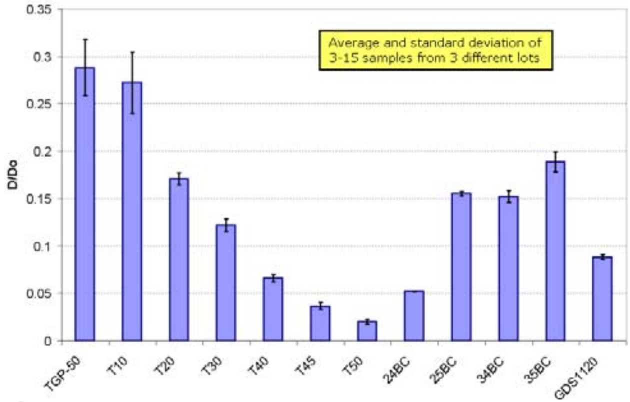
FY08-09 Plans and Milestones

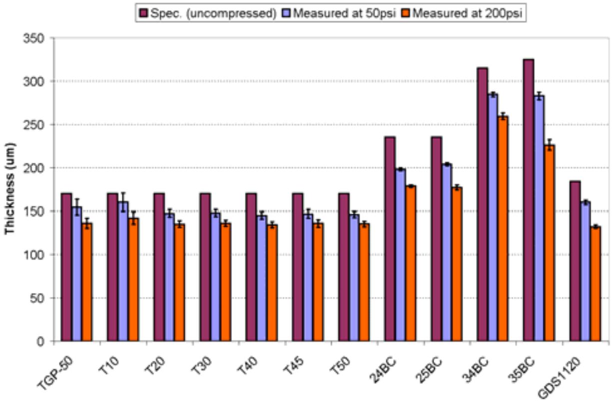
Month/Year	Milestone	Comments	% Complete
May 08	Ex-situ GDL materials characterization	Two-phase transport data limited, needs further analysis	100 %
Dec 08	GDL-Channel water transport experimental characterization	Initial data on model systems, GDL data delayed for increased channel studies	50%
May 09	LBM microscale model for two-phase flow	Development complete, testing and application underway	100%
Jun 09	Cell-scale water transport model implemented, component models validated	Ongoing, initial numerical issues resolved and experiments underway for channels. GDL-channel interface experiments and model treatment lagging	75%

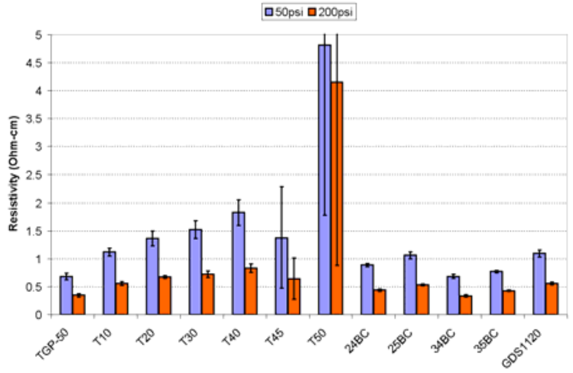
GDL Materials Characterization

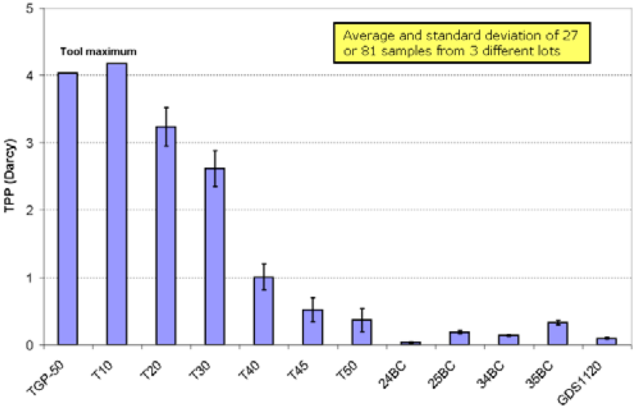












- **Key property database established for SGL, BMP & Toray papers with a range of PTFE loadings (Ballard, Techverse):**
  - **Porosity and Pore Size Distribution (MIP, MSP)**
  - **In- and Through-Plane Gas Permeability, Effective Diffusivity**
  - **Electrical and Thermal Conductivity**
  - **Thickness & Electrical Resistance Variation with Compression**

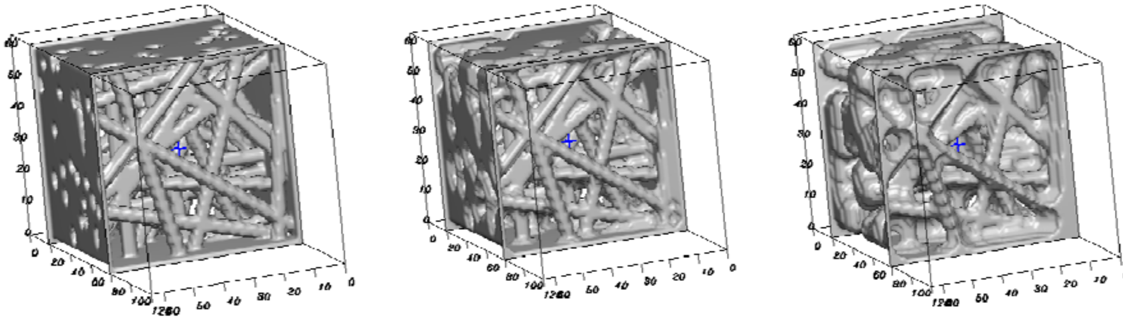
PTFE Effects on Gas Transport

Ballard Laser Scans

PTFE 0% **PTFE 20%** **PTFE 40%**

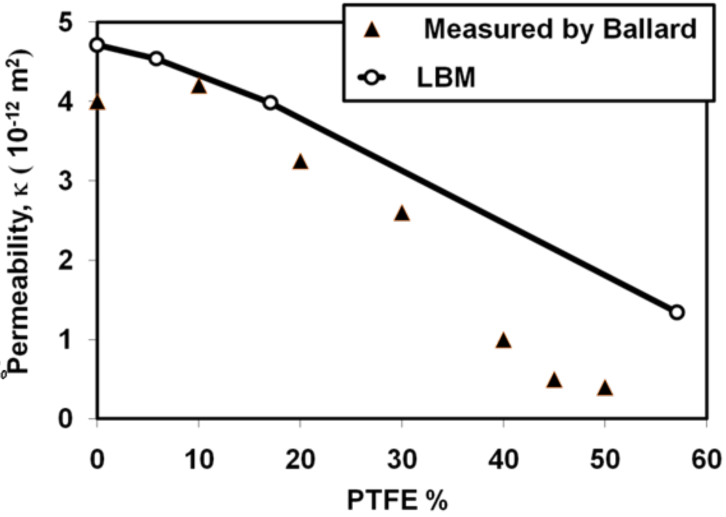
Laser scan images of Toray-050, Ballard Power Systems

Numerically Generated Microstructures for LBM



GDL microstructure reconstruction with Teflon® loading.

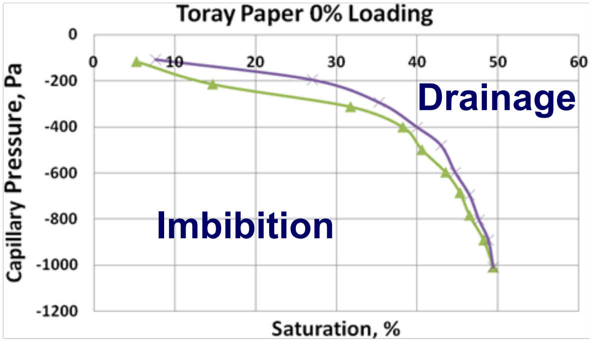
- PTFE distribution model developed from measured pore size distributions, laser scan images, and processing observations:
  - Teflon® solution is hydrophilic to carbon fibers.
  - Small pores and corner of larger openings are filled first.
  - Increase in fiber diameter due to Teflon® coating is negligible.

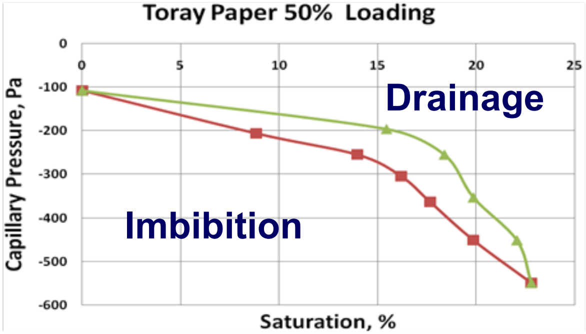


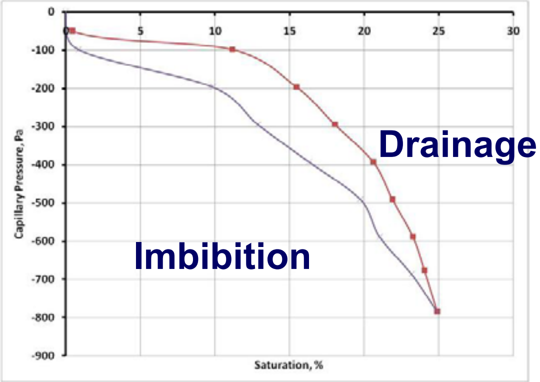
- Validates LBM for gas phase transport in GDL materials
- Verifies simple, stochastic microstructure generation approach is adequate for analysis of transport, PTFE loading effects in carbon paper GDLs
- IPP approximately linear in PTFE loading and porosity to 30% loading

Capillary Pressure and Residual Saturation

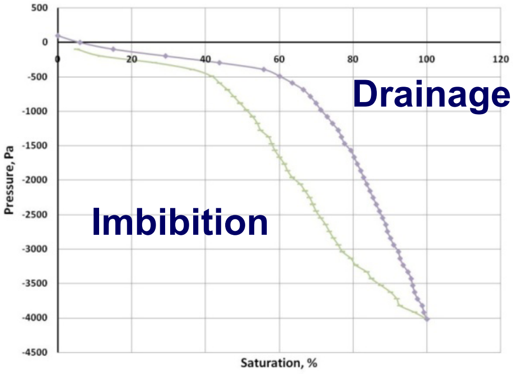
- **Positive Water Displacement technique, 90 mm diameter media for greater resolution**





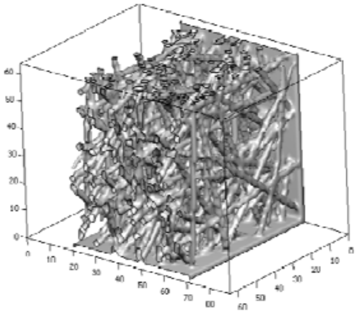


SGL 35 EC Media without (←) and with (→) porous Teflon® backing filter

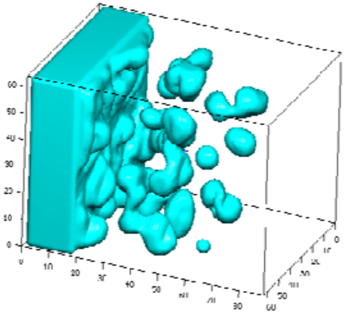


- **Techverse quantified breakthrough and residual saturation by volumetric and gravimetric analysis;**
  - **PTFE loading reduces saturation at breakthrough, not residual**
- **Addition of PTFE backing brings PC measurements closer to other reported ranges**
- **Greater hysteresis effect with increasing Teflon® content of media, weaker effect in Toray with no MPL**

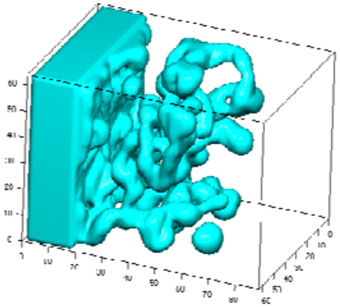
Capillary Pressure Simulation



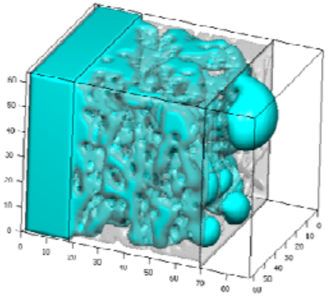
Toray-050



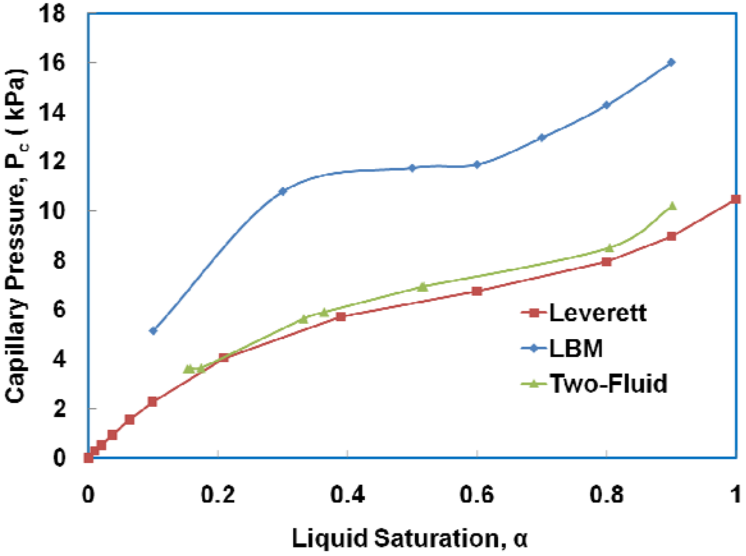
(a) α = 0.3,
dispersed globules

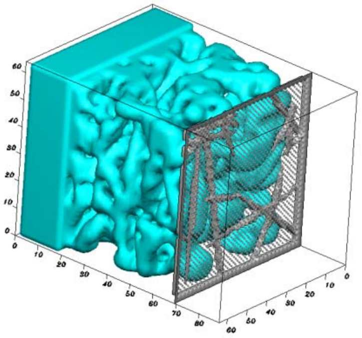


(b) α = 0.4,
interconnected streams



(c) α = 0.7,
droplet emergence





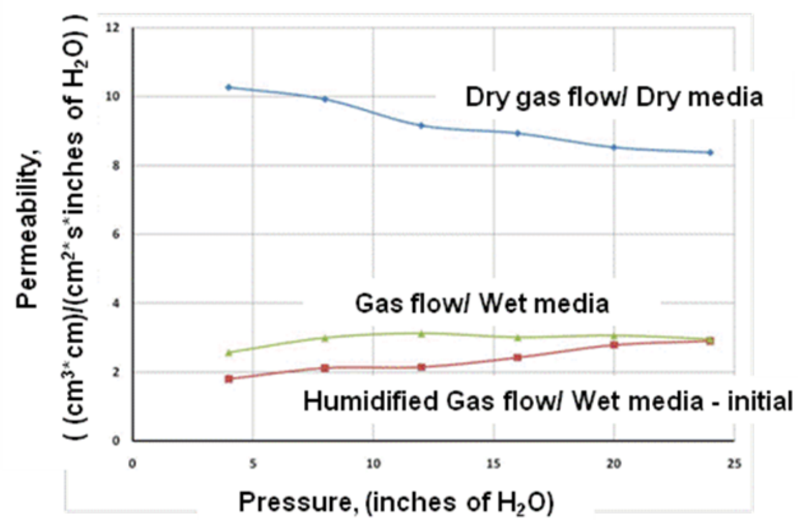
Hydrophobic porous plug to
prevent liquid escape from GDL.

α = 0.7

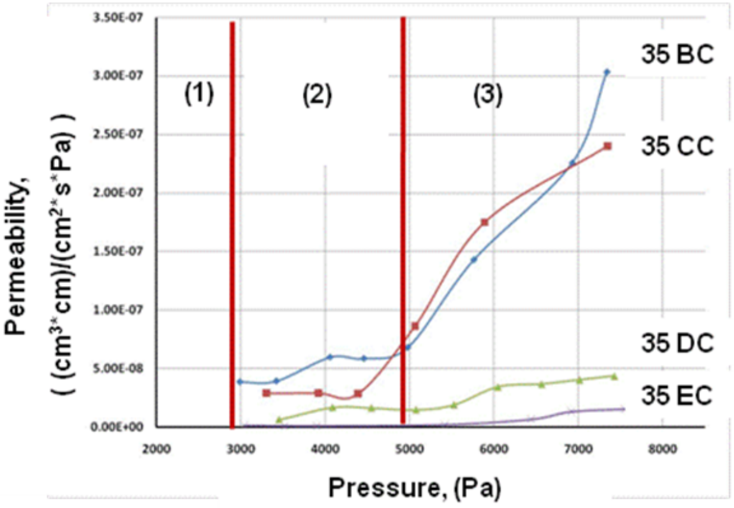
- Similar model definition, with water reservoir and hydrophobic 'frit', used to verify capillary pressure implementation in CFD-based two-fluid code
- LBM Results guided implementation details in CFD continuum model

Gas and Water Permeability in Wet GDLs

Gas Permeability in Wet Media



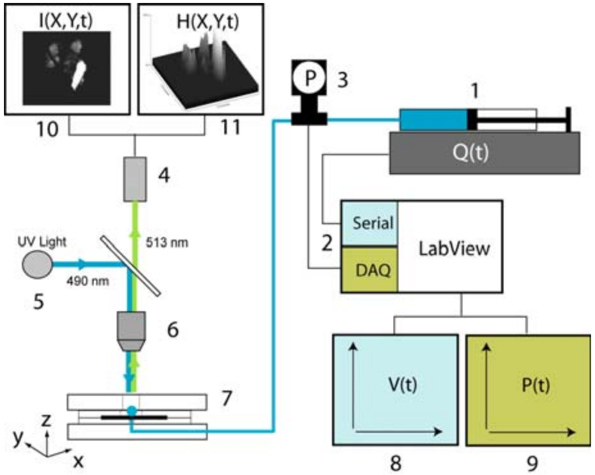
Water Permeability



- 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

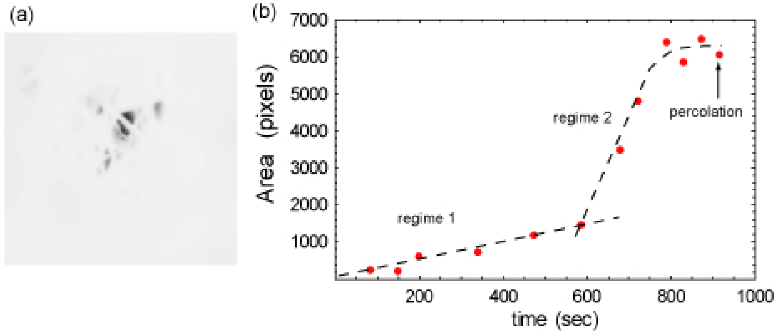
- Increasing PTFE content reduced water permeability
- Three distinct flow regimes.
  - 1: No flow. (below breakthrough pressure)
  - 2: Constant permeability. (moderate pressure)
  - 3: Increase in permeability with increased pressure, indicating opening of more channels for water flow

Transient GDL Water Transport Characterization and Modeling

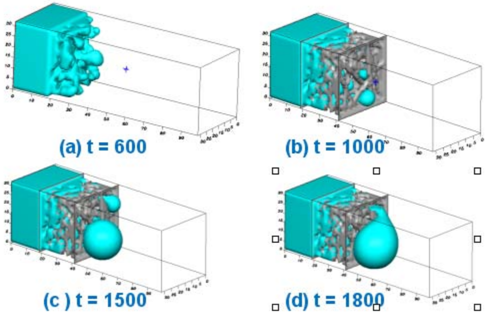


UVic is *Simultaneously* monitoring the development of the capillary flow, pressure, and volume injection rate of water percolating through the GDL porous layer

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



LBM Modelling of GDL Transport

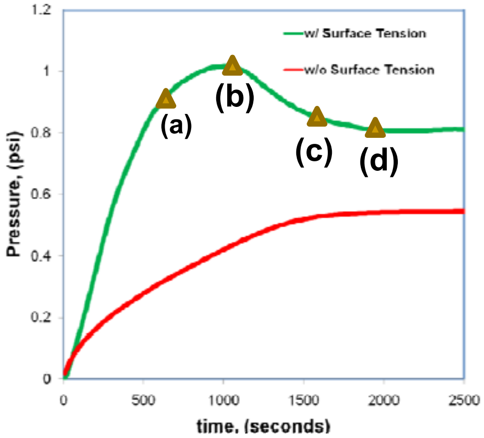

(a) t = 600

(b) t = 1000

(c) t = 1500

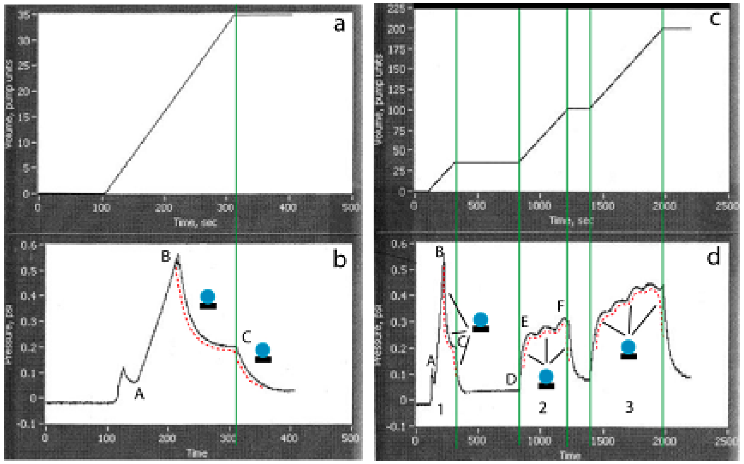
(d) t = 1800

Test GDL: porosity 0.75, thickness 100μm.



Dry sample: first breakthrough

Previously wet sample: continuous loading test

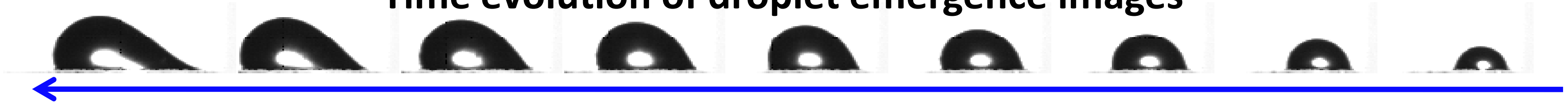


- Qualitative agreement, insight into under-surface transport
- Experiments and LBM guiding CFD model improvements

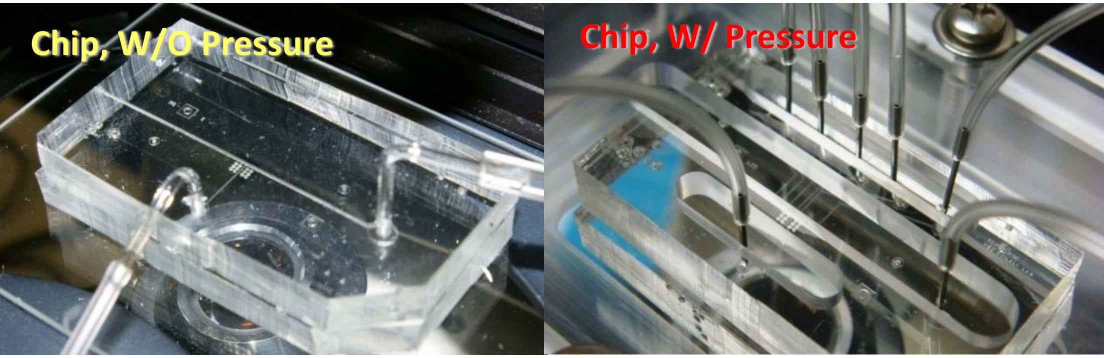
Invasion depends on history

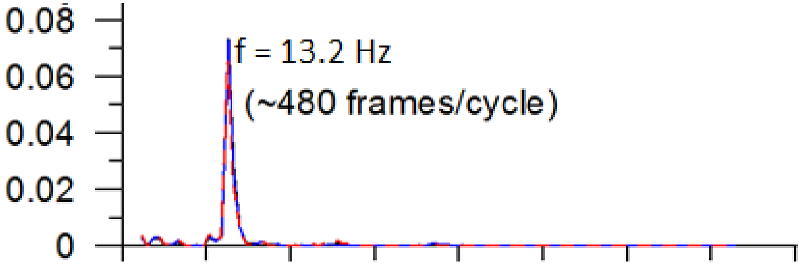
Droplet Emergence Analysis

Time evolution of droplet emergence images

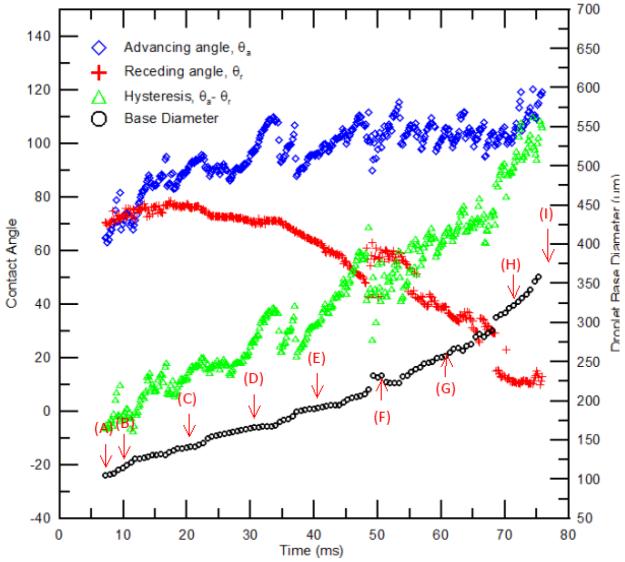


PDMS Chip and droplet dynamics studies at UVic for channel/GDL interface model

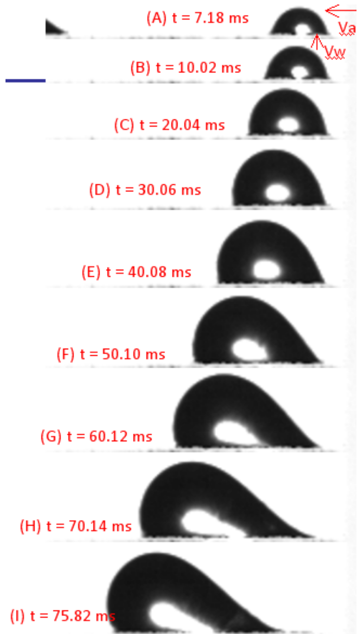




- **Image analysis for temporal correlation and FFT to quantify droplet emergence frequency**

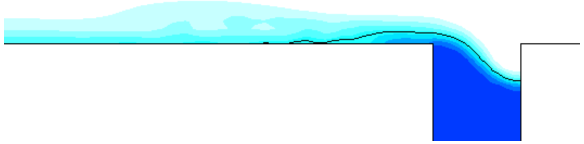


Dynamic Contact Angle Analysis



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

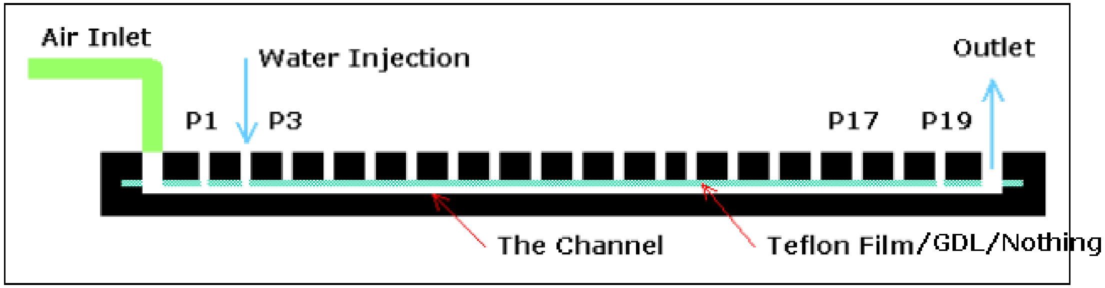
Initial Model Tests: Film/mist formation from drag overcomes surface tension



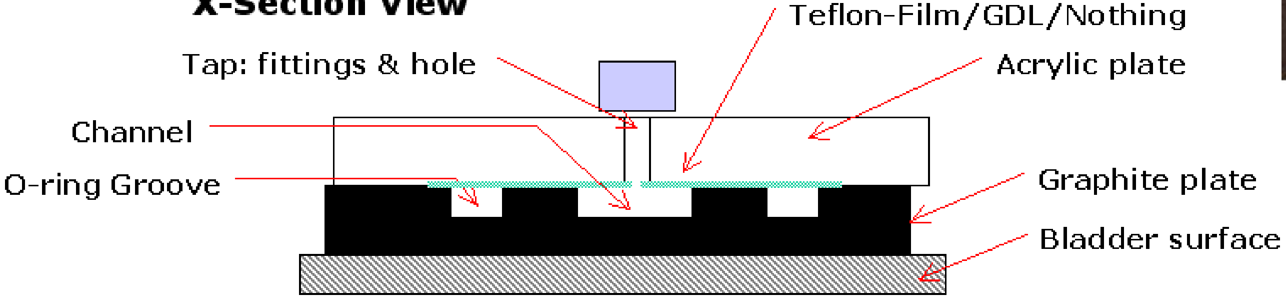
Ballard Two Phase Flow Channel DP Measurement

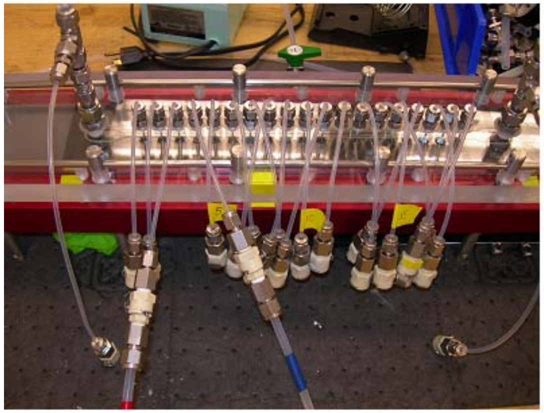
- **Interchangeable single channel graphite plates**
- **Nineteen pressure taps spaced 1.5cm apart (27cm total measurable length)**
- **Two phase pressure drop measured between taps 1 and 19 and water injected from tap 2**

Side View



X-Section View

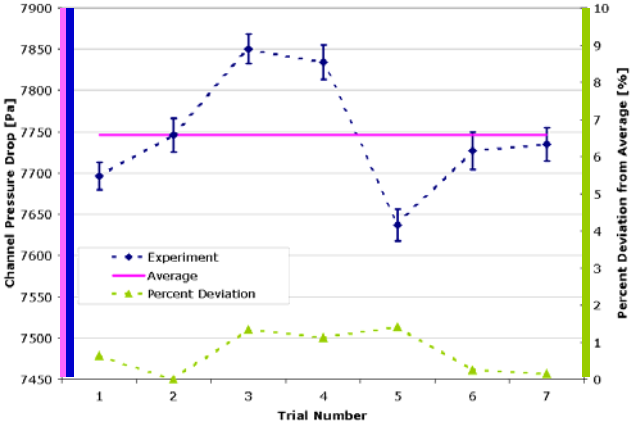




Two Phase Channel Model Validation Test Matrix

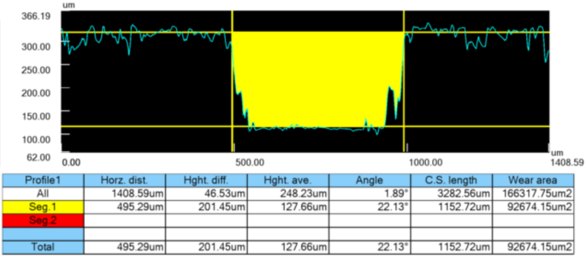
Current Density [A/cm^2]	Water Flow Rate [μL/min]	Temperature [C]	Outlet Pressure [bara]	Air Flow Rates [sccm]
0.3	**11**	**20**	**1.013**	**61, 204, 306, 407**
1	**37**	**20**	**1.013**	**61, 204, 306, 407**
1.5	**56**	**20**	**1.013**	**61, 204, 306, 407**
2	**75**	**20**	**1.013**	**61, 204, 306, 407**

Experimental error estimation

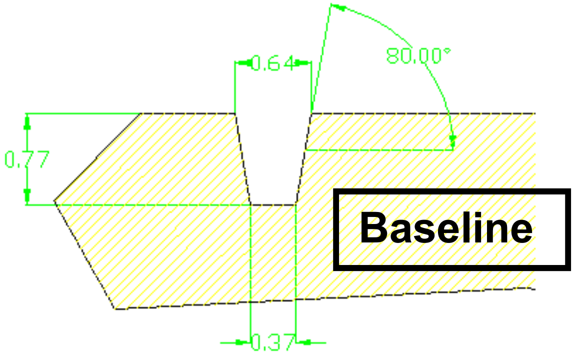


407 sccm, 37 mL/min

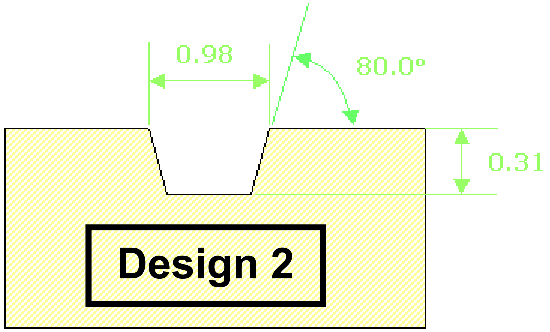
Keyence microscope assessment of micro-channel machining accuracy (within 10 μm)



Profile1	Horz. dist.	Hght. diff.	Hght. ave.	Angle	C.S. length	Wear area
All	1408.59um	46.53um	248.23um	1.89°	3282.56um	166317.75um2
Seg.1	495.29um	201.45um	127.66um	22.13°	1152.72um	92674.15um2
Seg.2						
Total	495.29um	201.45um	127.66um	22.13°	1152.72um	92674.15um2

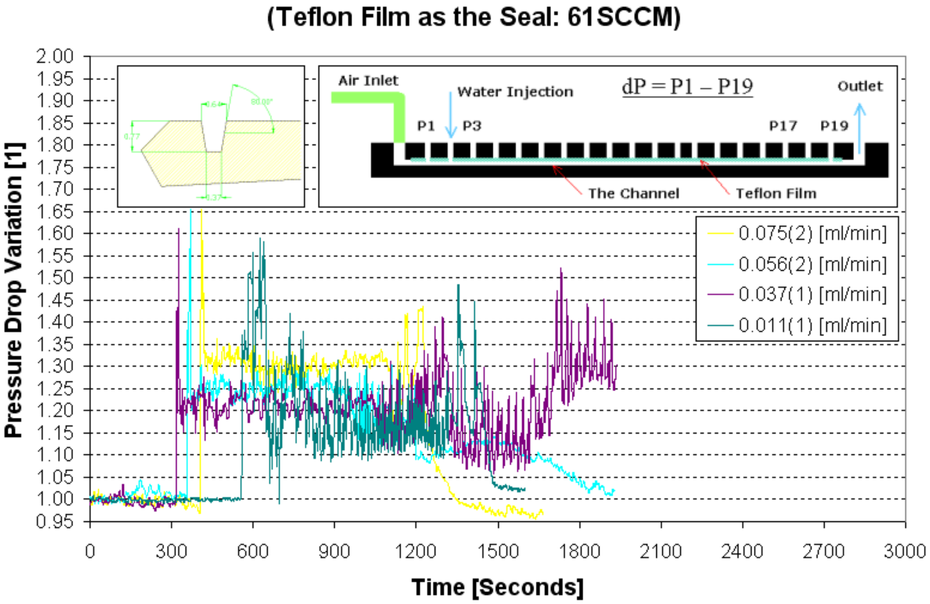


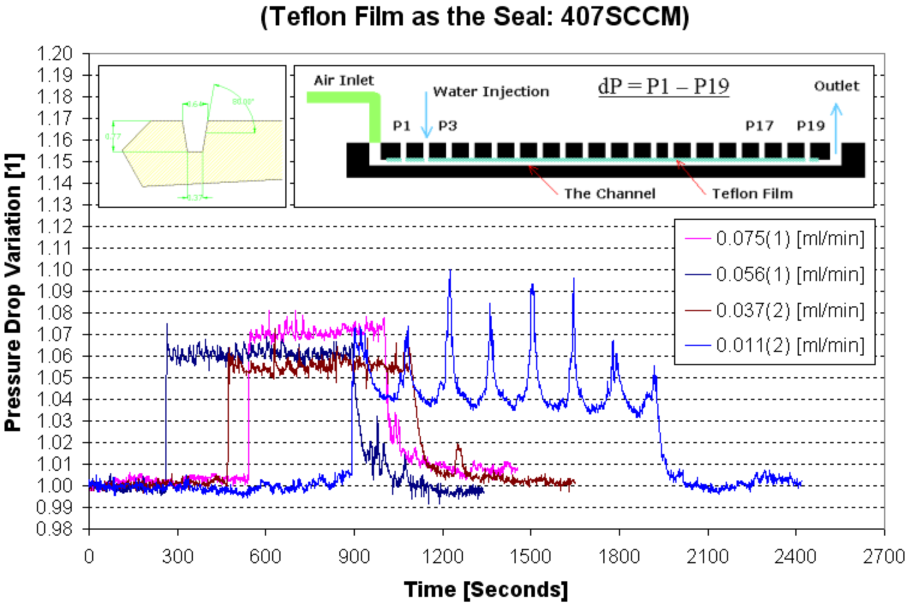
Baseline



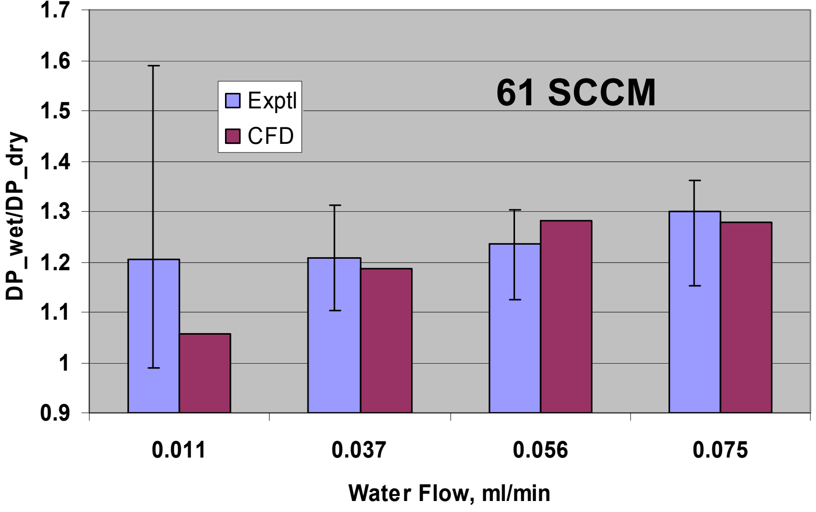
Design 2

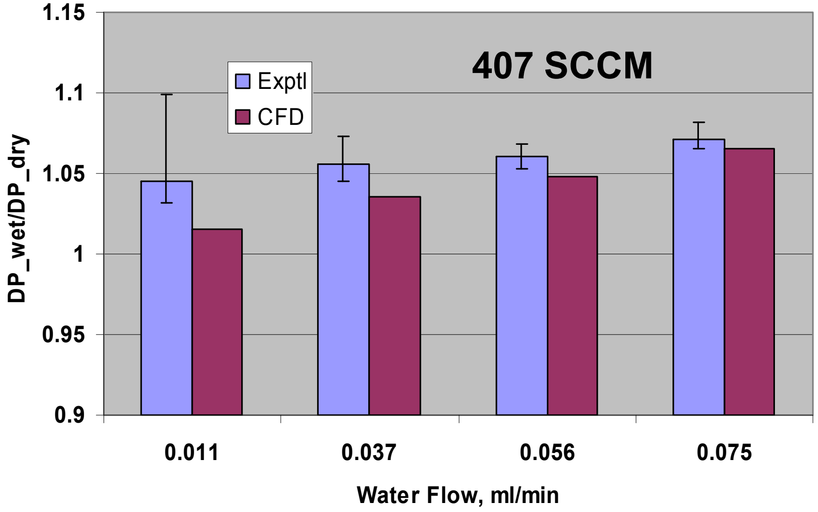
CFD Pressure Drop Validation with Water Flow Rate



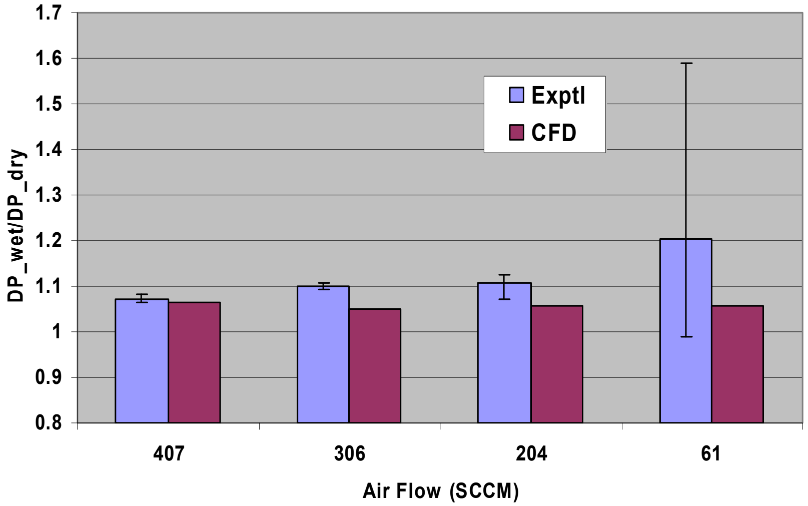


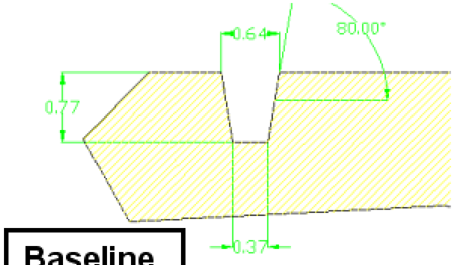
- Steady two-phase CFD captured trends with water flow rate
- Experimental repeatability worse at low water and low air



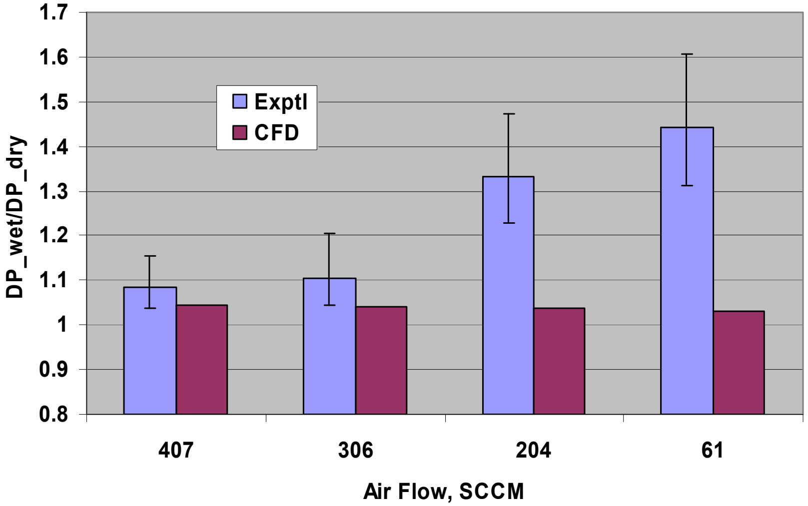


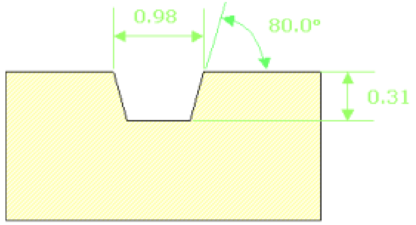
CFD Testing with Total Flow, Design





Baseline





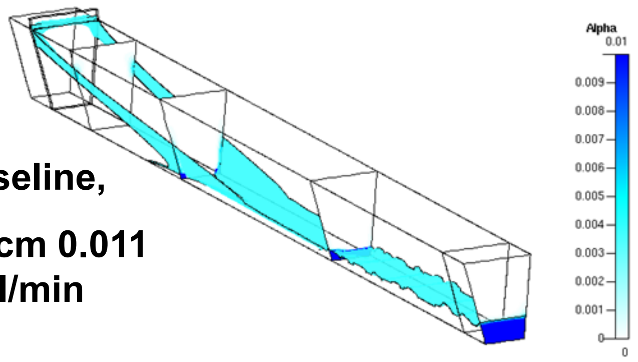
Design 2

- 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

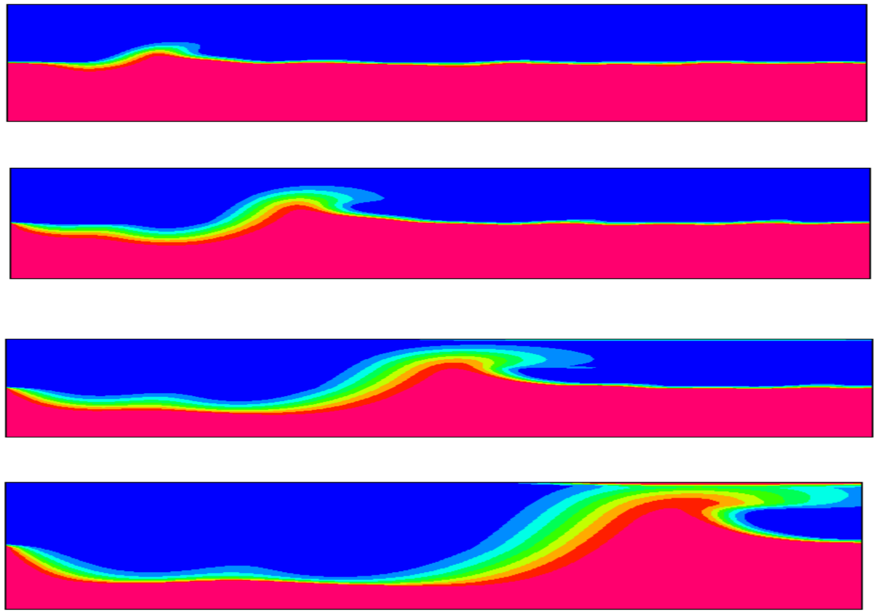
Stratified, Wavy Flow Verification

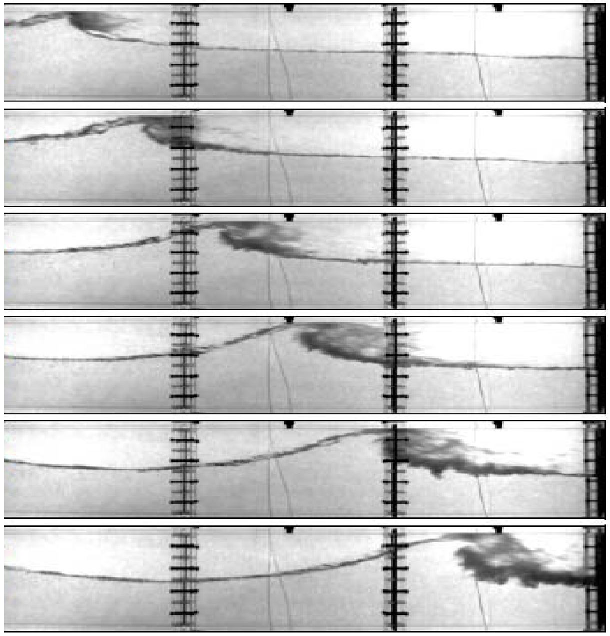
Baseline,

61 sccm 0.011 ml/min



Lower gas velocities transfer less momentum to the water, film falls to bottom due to gravity

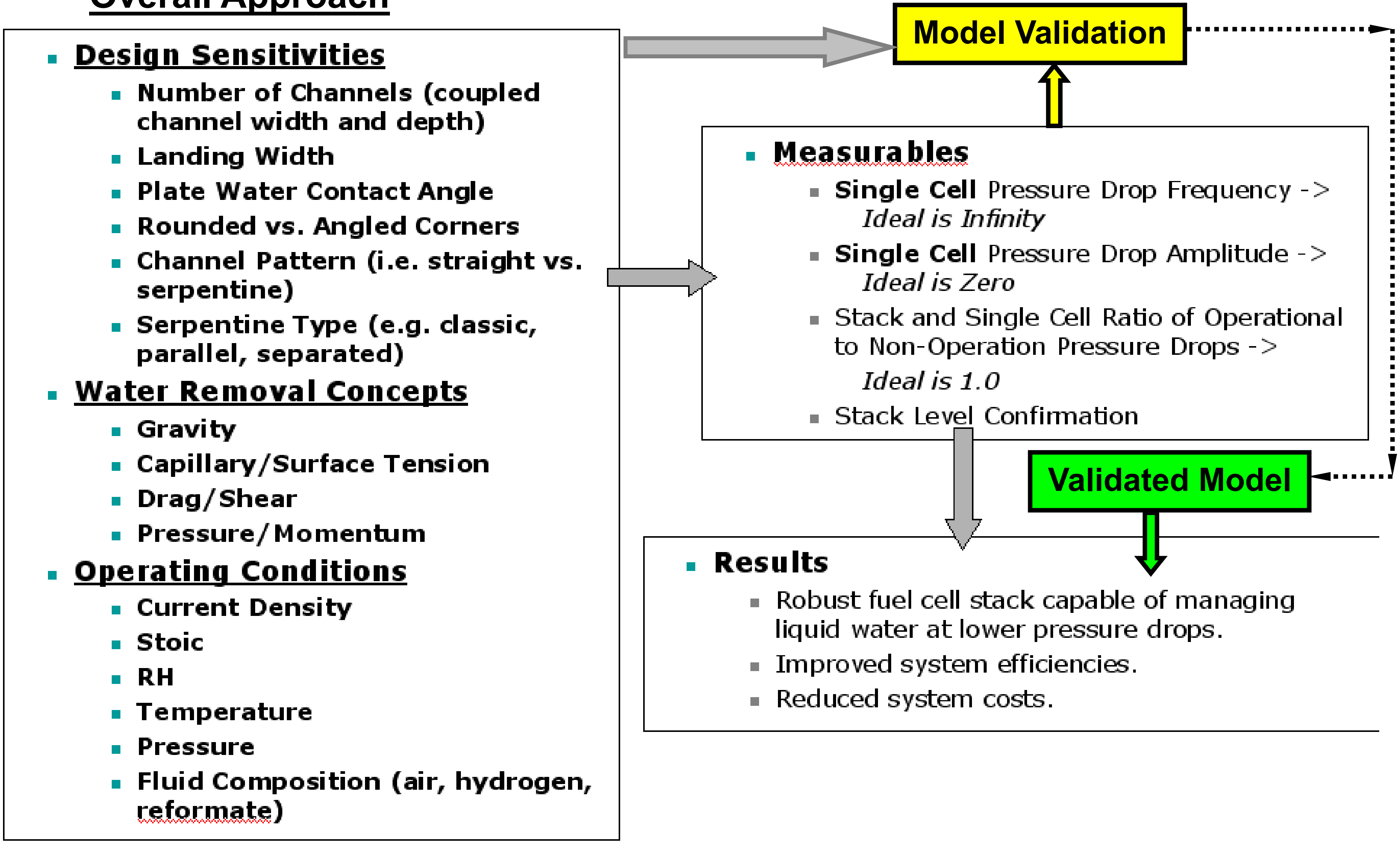




- ESI achieved qualitative agreement with experiment for slug behavior in a stratified two-phase channel flow (0.69 m/sec water, 2.2 m/sec air, 50x250 mm)
- Requires transient to capture dynamics, investigating approaches to reduce computational expense

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)**

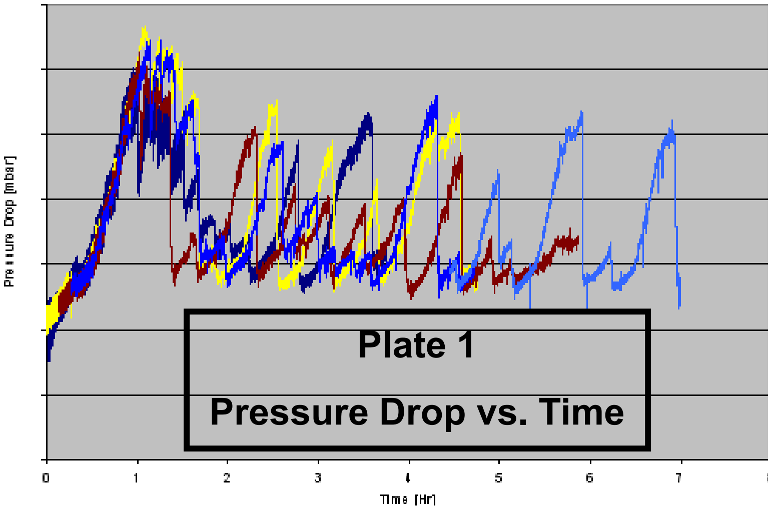
Model Validation

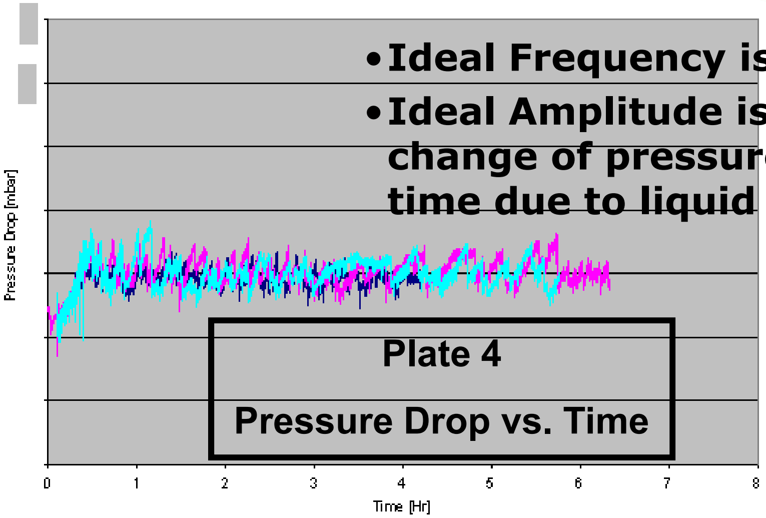
- **Measurables**
  - **Single Cell** Pressure Drop Frequency -> *Ideal is Infinity*
  - **Single Cell** Pressure Drop Amplitude -> *Ideal is Zero*
  - Stack and Single Cell Ratio of Operational to Non-Operation Pressure Drops -> *Ideal is 1.0*
  - Stack Level Confirmation

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**

- **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**

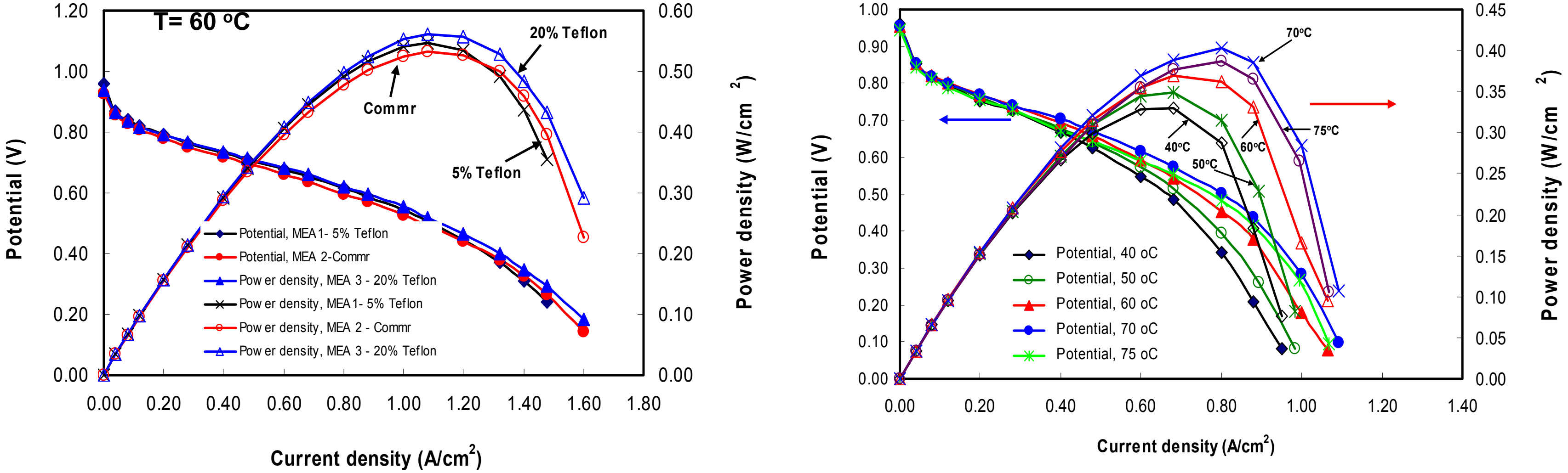
Plate	Pressure Drop Amplitude Relative to Plate 1	Pressure Drop Frequency (Hz)
1	1.0	~6e-4
4	0.27	~15e-4

- **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**

Single Cell Performance Characterization

BCS Fuel Cells, Inc.

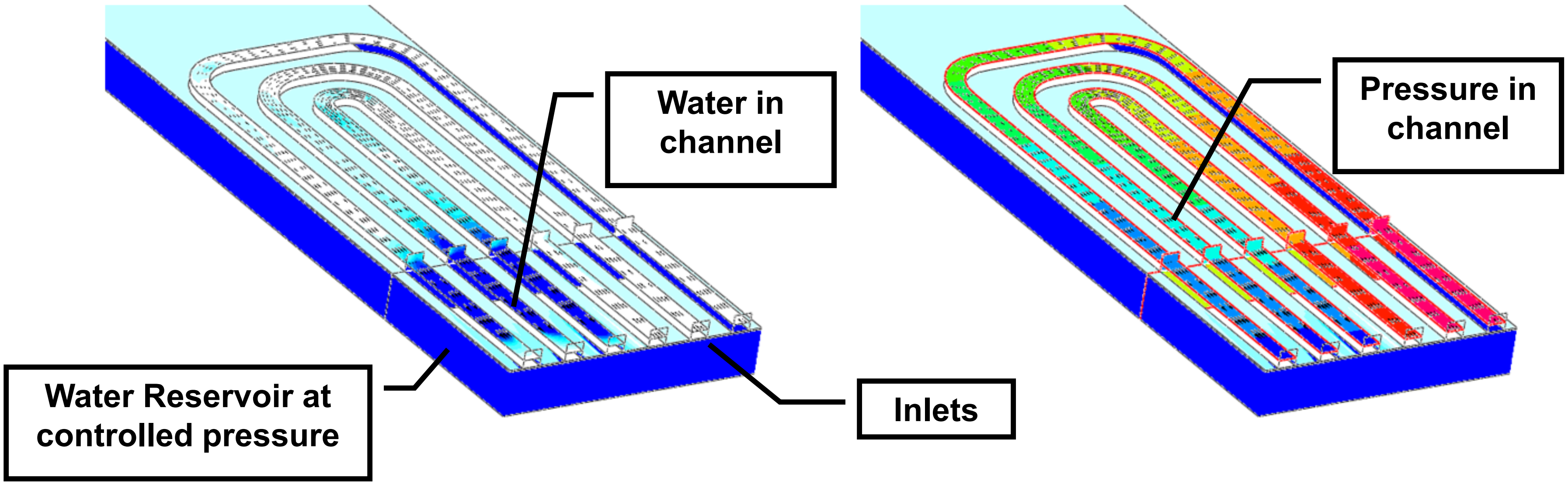
Air stoic.: 1.75, Air pressure: 8 psig, H_2 pressure: 3 psig, Anode 0.2 mg/cm² Pt, Cathode: 0.5 mg/cm² Pt



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**

GDL Water Permeation into Channel



- 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