# 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: FC34


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# Overview

- **Timeline**
  - Start Date: 6/1/07
  - End Date: 5/31/11
  - Percent Complete: 18%
- **Budget:**
  - Total Project Funding:
    - DOE $4,900K
    - Contractors $1,500K
  - Funding Received in FY07
    - $790K
  - Funding for FY08
    - $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
  - Research Triangle Institute
  - SGL Carbon
  - U. Victoria

# Water Management & Performance

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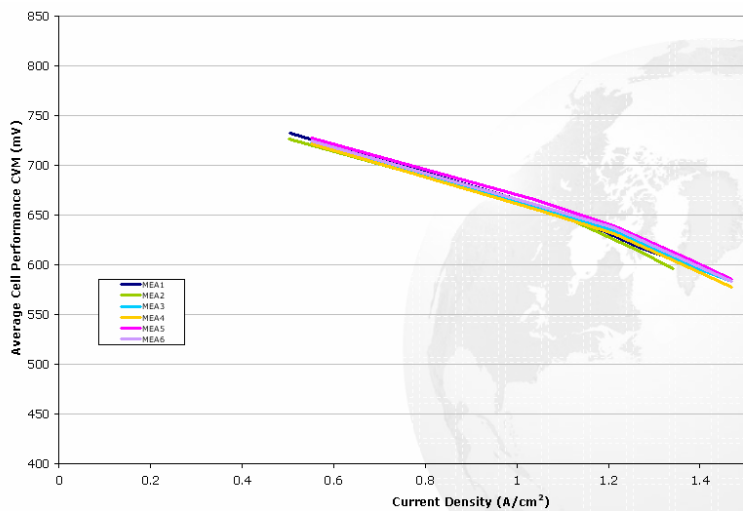
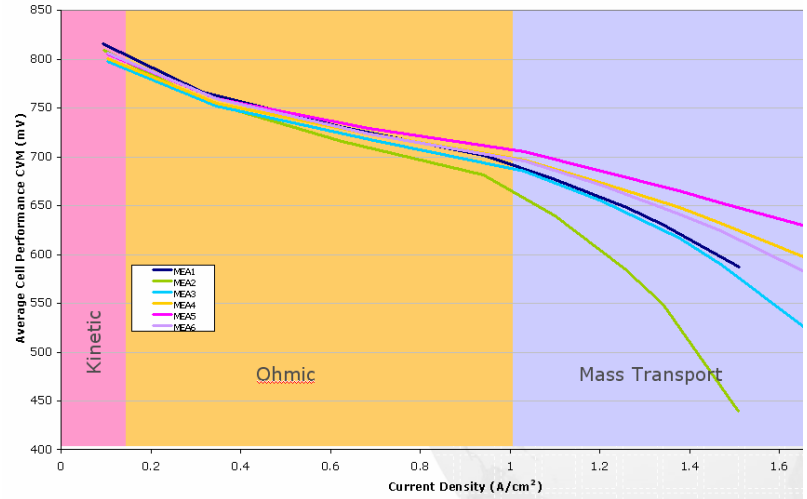
DRY OPERATION




WET OPERATION




- **Several different MEAs, with different GDL properties and Teflon loadings, perform nearly identically with a given flow field when operated relatively dry, but show markedly different performance above 1 A/cm$^2$ under relatively wet conditions**
- **Additionally, some flow field designs are better at managing water for a given MEA**

Optimized water management is key for performance improvements and is the main focus of this project

# Program Objectives

- **Overall:**
  - **Develop advanced physical models and conduct material and cell characterization experiments;**
  - **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 models in a commercial modeling and analysis tool.**
- **FY 2007 and 2008:**
  - **Perform baseline characterization for Gas Diffusion Layer (GDL) materials => two-phase transport relevant properties**
  - **Develop procedures for, and begin gathering, cell- and stack-level diagnostic data**
  - **Down-select model formulations, implement, and test improved models for transport in GDLs, channels, and across interfaces**

# Milestones

| Month-Year | Milestone or Go / No-Go Description |
|---|---|
| Sep-07 | Milestone: Compilation of initial in-situ diagnostic data package and assessment of cell-scale modeling capabilities (Ballard, CFDRC) |
| Jun-08 | Milestone: Down-select and implement framework for improved water transport models in cell-scale models (ESI, CFDRC, Ballard) |
| Jun-08 | Milestone: Develop internal resistance measurement technique for self-humidified cell diagnostics, verify method is capable of identifying flooding onset (BCS) |
| Jun-08 | Milestone: Baseline GDL material characterization for physical properties (porosity, microstructure), transport properties including permeability and capillary pressure (RTI, Ballard) |
| Jun-08 | Milestone and Go/No-Go: Complete initial development of Lattice Boltzmann Method for single-phase flows, verify model against benchmark test cases (CFDRC, ESI) |

# Approach

- **Overall:**
  - Integrated experimental characterization and model development
  - Systematically address each of the component regions of the cell
  - Apply resulting understanding and predictive capabilities to improve water management

- **Modeling Approach:**
  - Develop advanced models, and determine model parameters, for water transport 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

# Experimental Validation Data

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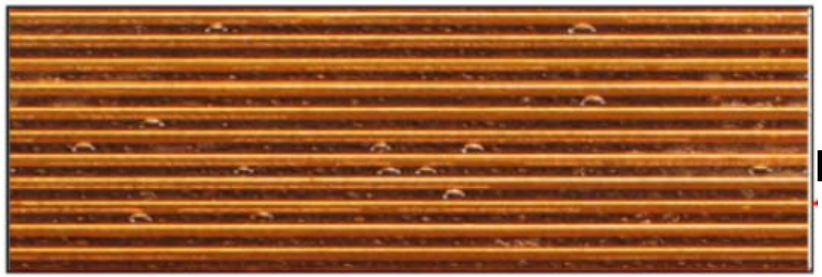
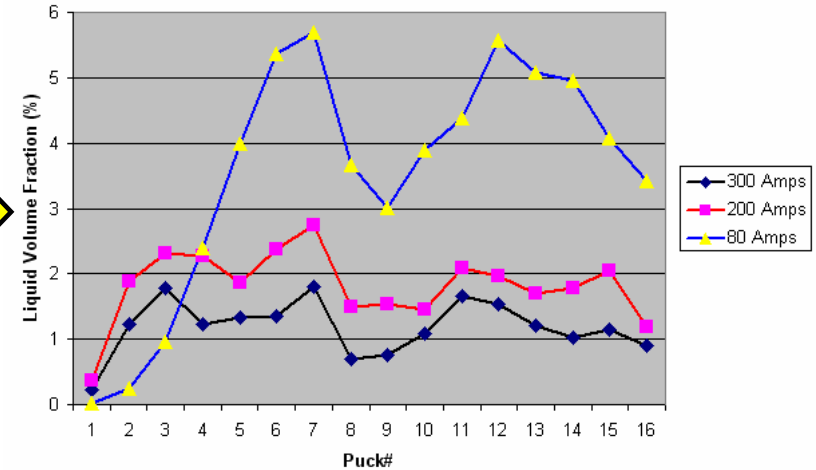
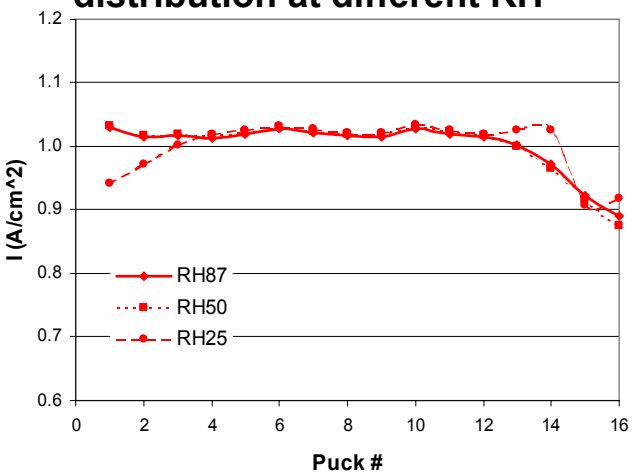
**FlowViz for liquid water measurement in channels of an operating cell**



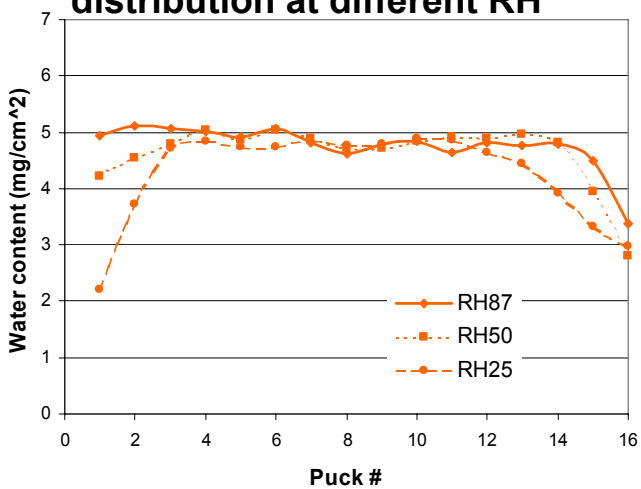
**Measured liquid water volume fractions in channels at 16 pucks along the cell**




**Cell diagnostics data – current distribution at different RH**




**Cell diagnostics data – MEA water distribution at different RH**



# Unit Cell Model Assessment

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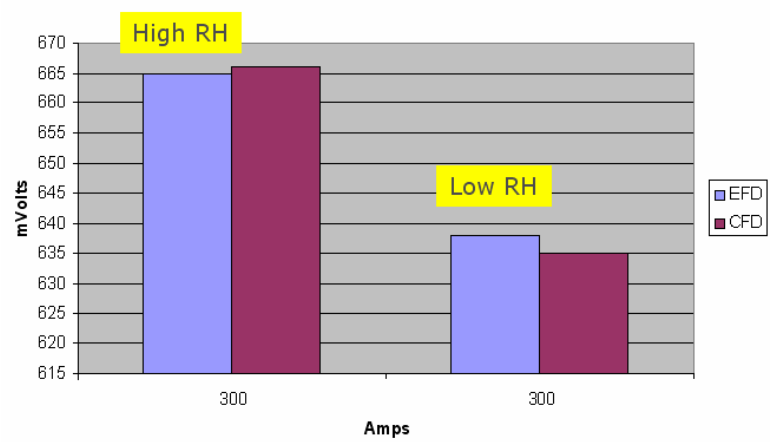
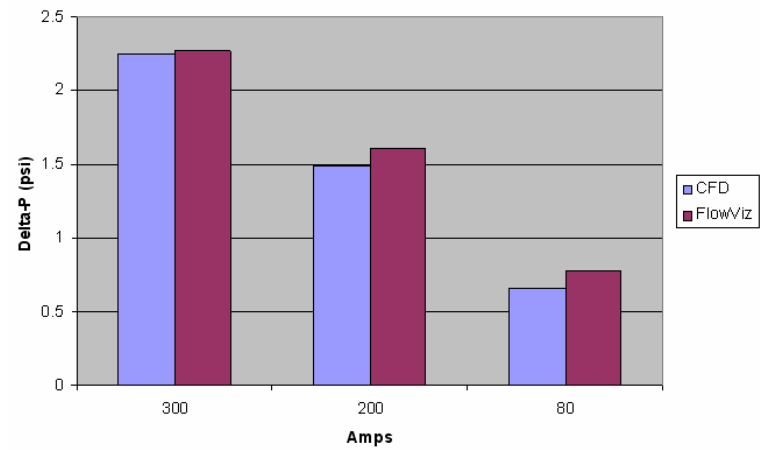
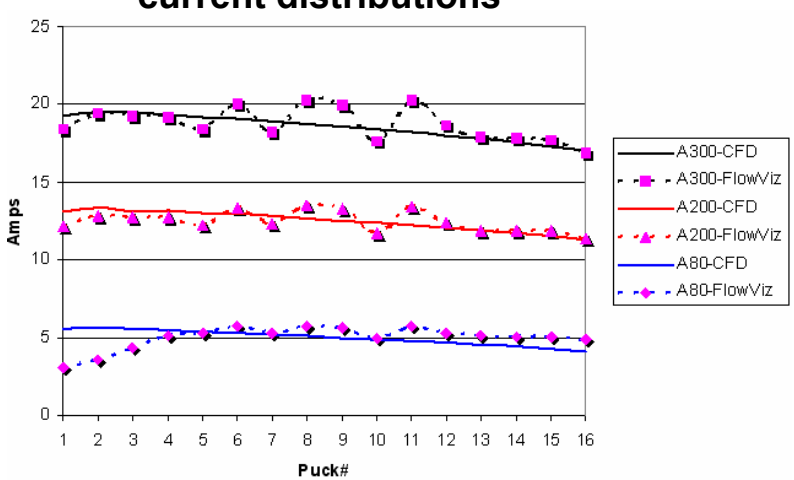
### Measured vs Predicted cell performance at different RH



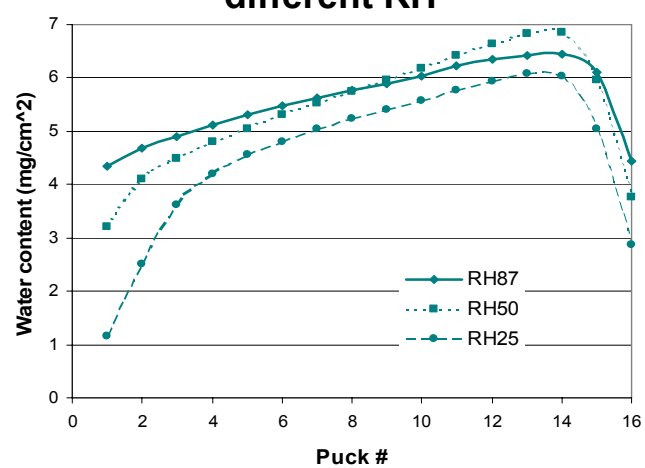

### Measured vs Predicted wet pressure drop in cell at different currents




### Measured vs Predicted current distributions




### Predicted MEA water at different RH



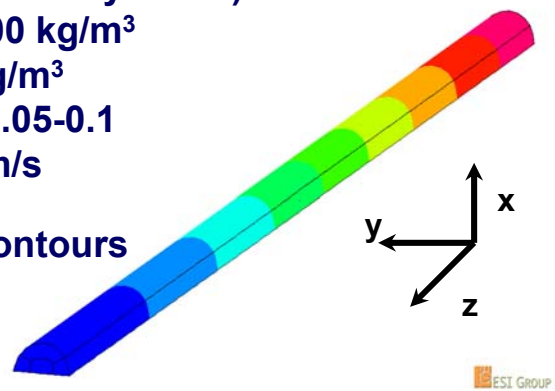
# Cell Scale Model Improvements

ESI GROUP
THE VIRTUAL TRY-OUT SPACE® COMPANY

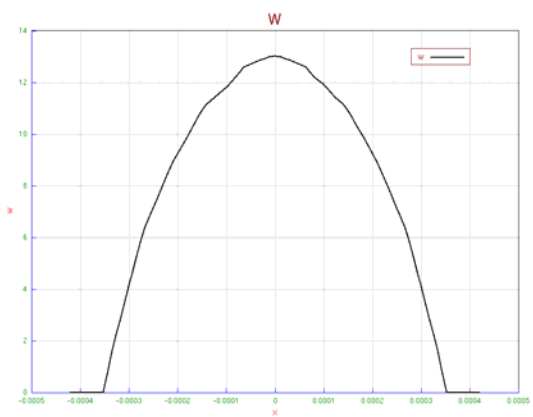
CFDRC

**Cathode Channel (Ballard Systems)**
- Liquid Density = 1000 kg/m$^3$
- Gas Density = 3.3 kg/m$^3$
- Volume-Fraction = 0.05-0.1
- Inlet Velocity = 6.5 m/s

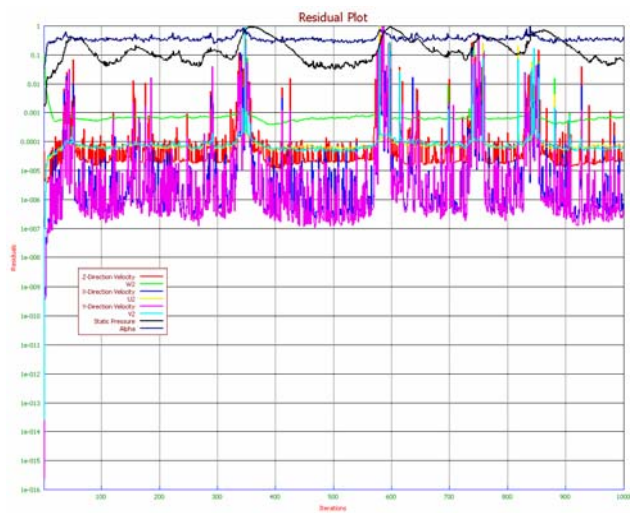
**Pressure Contours**



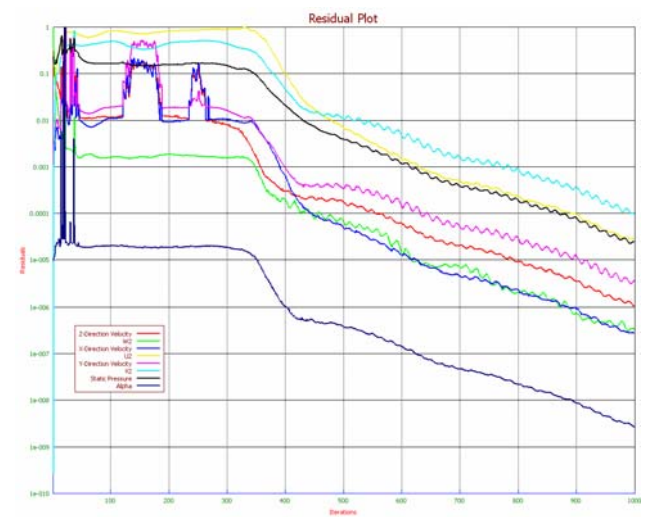

- **Selected true two-phase flow treatment as transport formulation**
- **Extended two-phase flow to address porous media**
- **Improved convergence and robustness for two-phase flow analysis of channels**




**Axial (z) Velocity vs. Radial Position (x)**




**Formulation (A)**

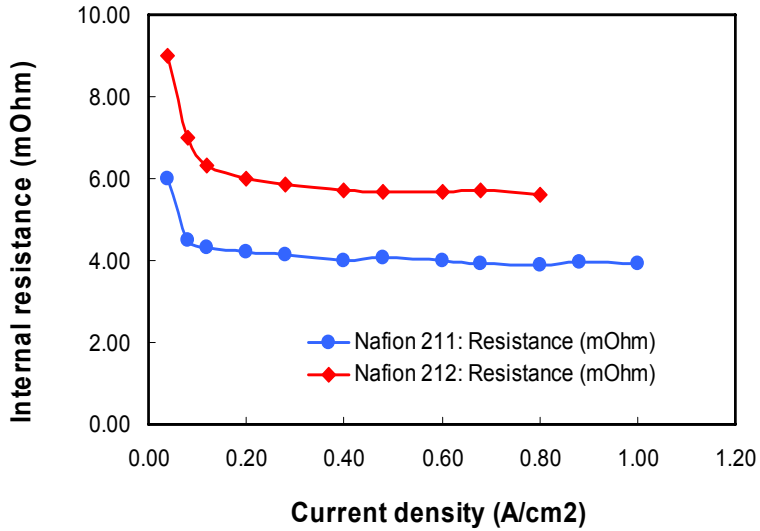


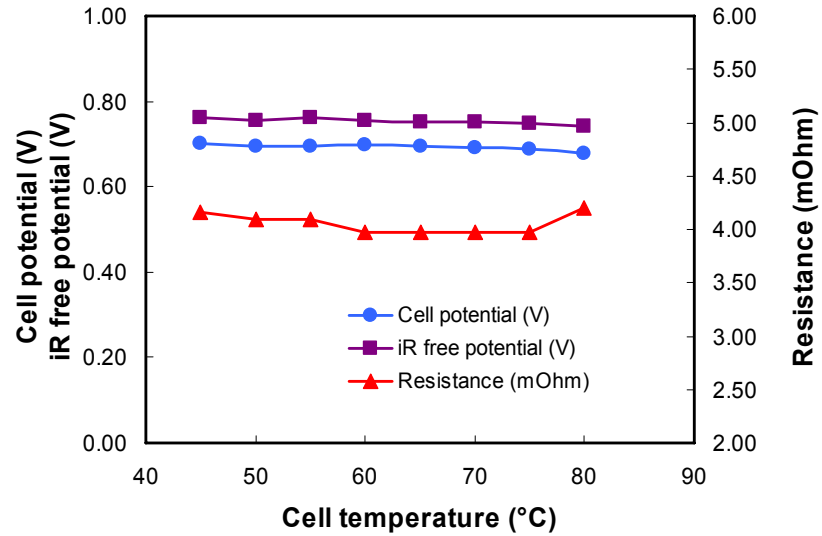

**Formulation (B)**

**Convergence Plots**

# Self-Humidified Cell Diagnostics

## BCS Fuel Cells, Inc

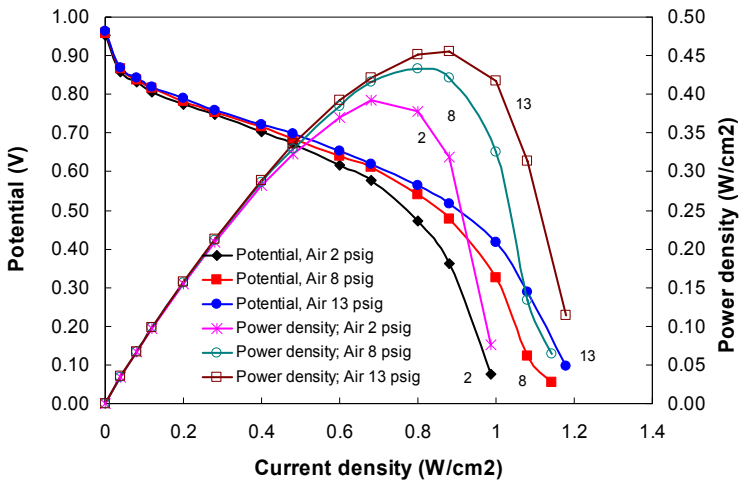


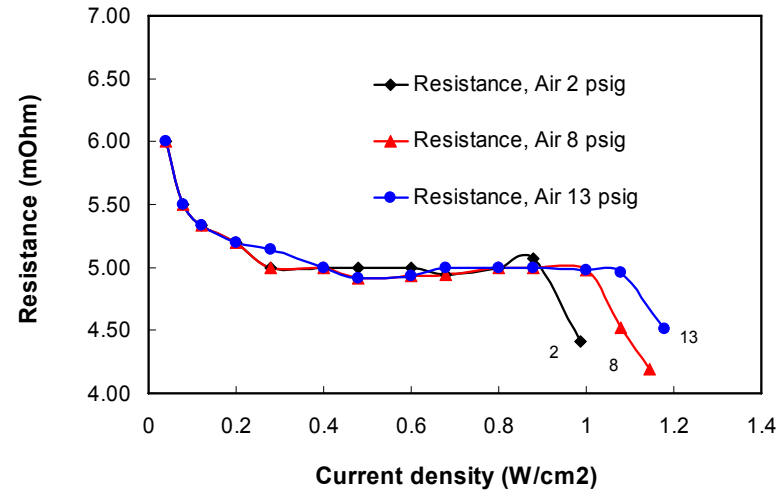




- **Established current interruption based Internal Resistance, IR, drop measurement technique in single cells**
  - **Measured IR with membranes Nafion 211 and 212, the expected distinct differences in cell resistance are observed**
  - **Single cell IR using Nafion 211 membrane drops with increasing T as expected. Beyond 70° – 75°C rises indicating limit of self-humidification in the cell.**
- **Enables diagnostics of self-humidification, and analysis of materials effects, to guide performance improvements**

# S-H Cell Flooding Detection

## BCS Fuel Cells, Inc




**Effect of air pressure on cell performance and resistance:**

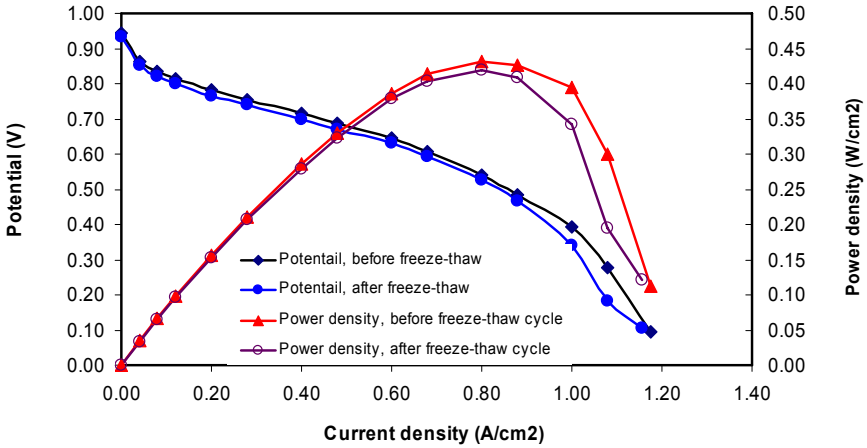
**Air stoic: 1.25; Temp: 40 °C; H2 pressure: 2 psig, Anode 0.2 mg/cm² Pt, Cathode 0.5 mg/cm² Pt**

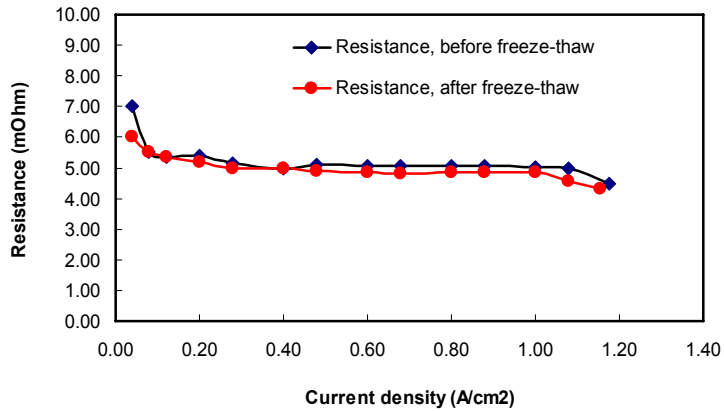
- **Established detection of accelerated electrode flooding using GDL with low Teflon content, 5%, in the micro-porous layer (MPL)**
  - **Plot shows V-I and W-I data extending to extreme mass transfer control (EMTC) regime**
  - **A sudden or sometime a gradual drop in IR in the EMTC region is indicative of the initiation of electrode flooding.**
- **Correlation of internal resistance with flooding has not been previously reported. IR monitoring is a promising, simple technique for in-situ detection of electrode flooding with potential application to active control and cell-scale model validation**

# S-H Cell Freeze-Thaw Cycling

## BCS Fuel Cells, Inc

**Air stoic: 1.25; Temp: 40 °C; H2 pressure: 2 psig, Air Pressure 8 psig**




- **Initiated Freeze-Thaw Cycle (F-TC) tests in single cells to study the effect on performance and electrode flooding behavior. Cell frozen to -20°C, 6 cycles**
- **Cell performance slightly drops with F-TC, internal resistance drop at high currents indicates electrode flooding before and after cycling**
- **After F-TC both performance and resistance drop slightly, indicating a possible internal structural change of electrodes surface and/or MEA matrix. Work is in progress to investigate these issues in single cells and stacks**

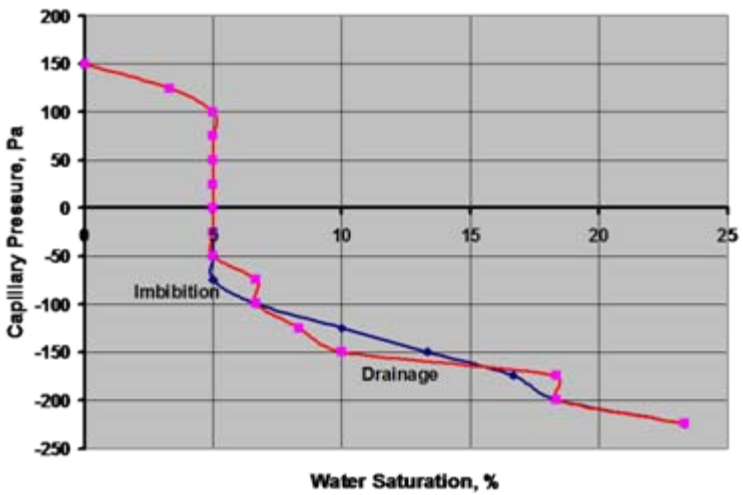
# GDL Capillary Pressure

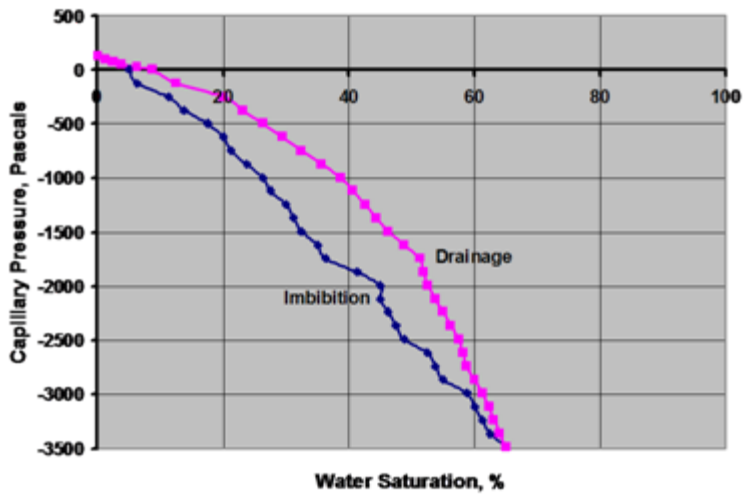
SGL GROUP THE CARBON COMPANY

RTI INTERNATIONAL

| 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 |

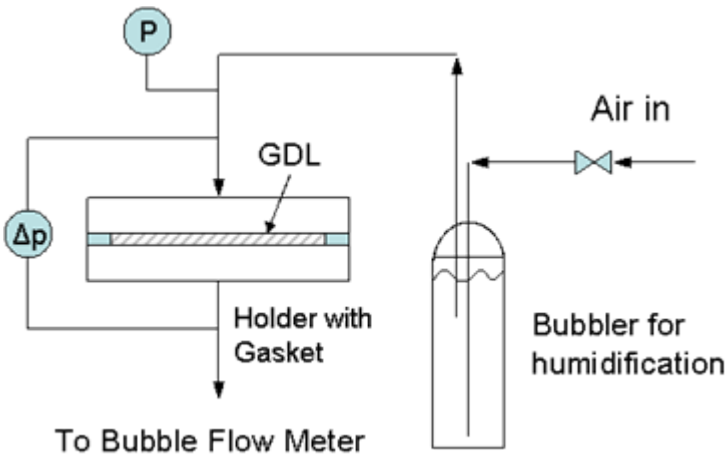
- **Positive Water Displacement technique**
  - **90 mm diameter media for greater resolution in water uptake measurements**
- **Water breakthrough observed at isolated locations on GDL surface limiting water saturation of media**
- **Characterizing SGL provided materials**
  - **Series 24, 25, 34, and 35**



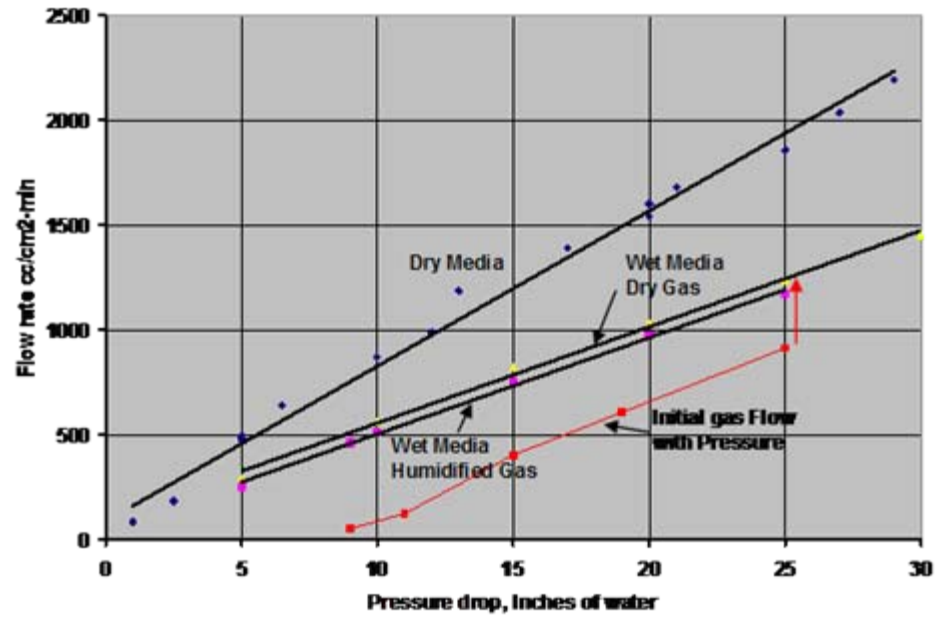

- **SGL 24 BC – 218 µm:**
  - **Coarser pore size, thinner media**
  - **No hysterisis behavior**
  - **Quick breakthrough at low ΔP**
- **SGL 35 BC – 321 µm:**
  - **Finer pore size thicker media**
  - **Hysterisis in imbibition/drainage**
  - **Need high ΔP for breakthrough**

# Gas Permeability of Dry/Wet GDL




Permeability Flow Apparatus

**SGL 35BC Wet Permeability Characterization**




- **Dry permeability with dry GDL**
- **For wet permeability GDL is initially filled with water under pressure, gas flow used to expel part of the water (red curve in figure)**
- **Very little difference in wet permeability of GDL with dry gas or humidified gas.**
- **Gas flow primarily occurs through voids opened by water expelled from media with gas ΔP across the media**

# GDL Microstructure Characterization

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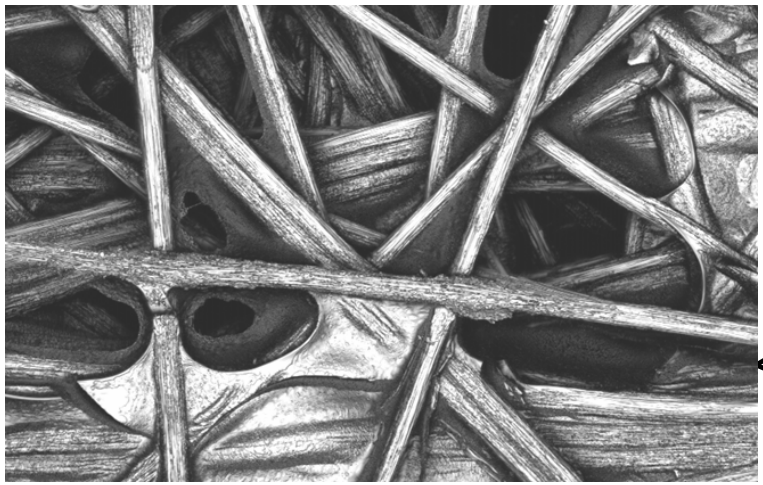
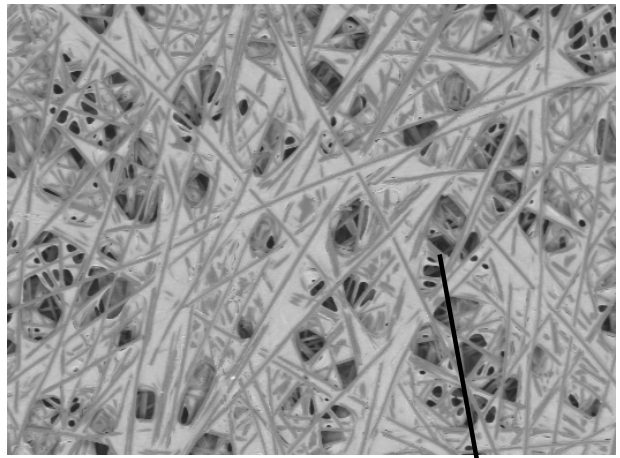
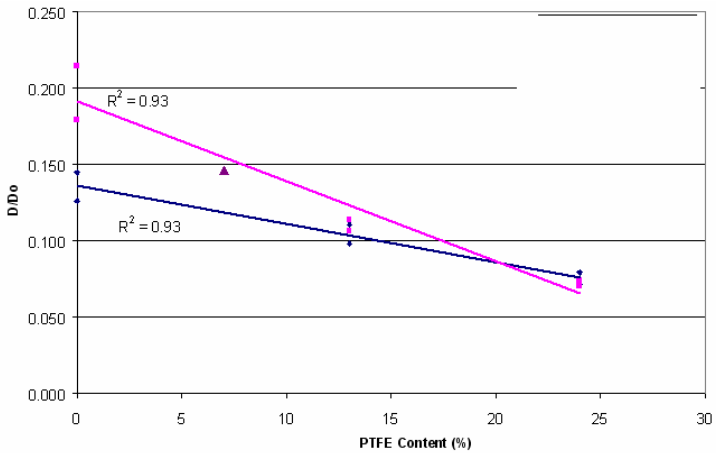
**Laser Microscope imaging of a teflonated GDL for structure**

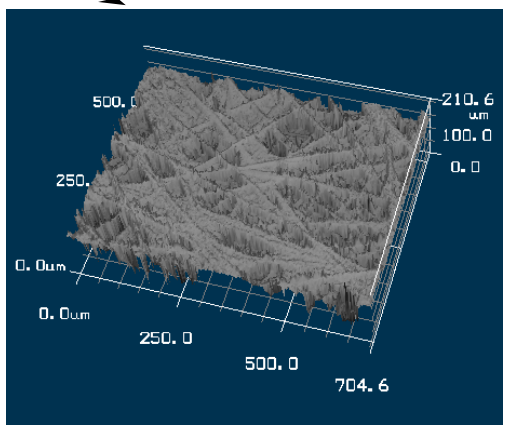


**SEM imaging to identify teflon**

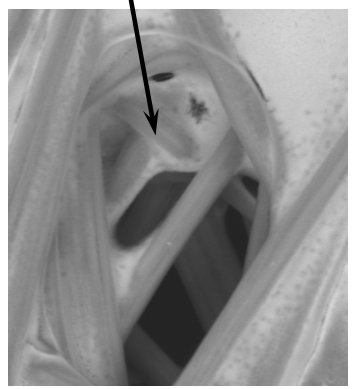


**D/Do (diffusivity ratio) characterization wrt teflon loading for different GDLs**



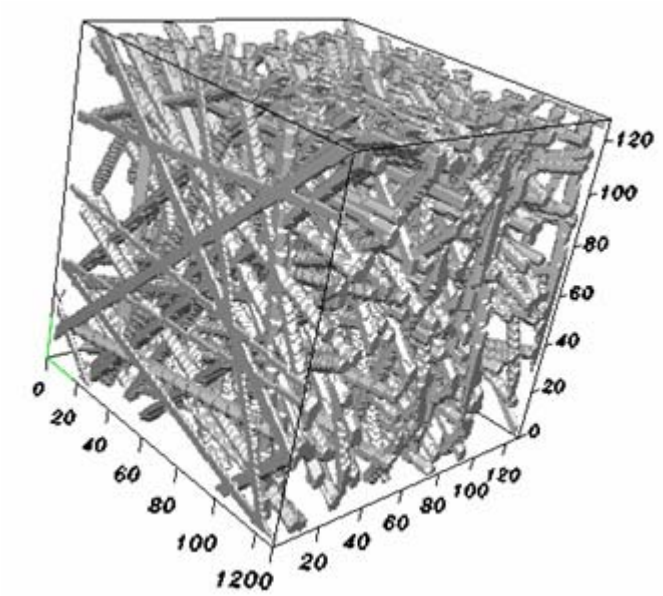



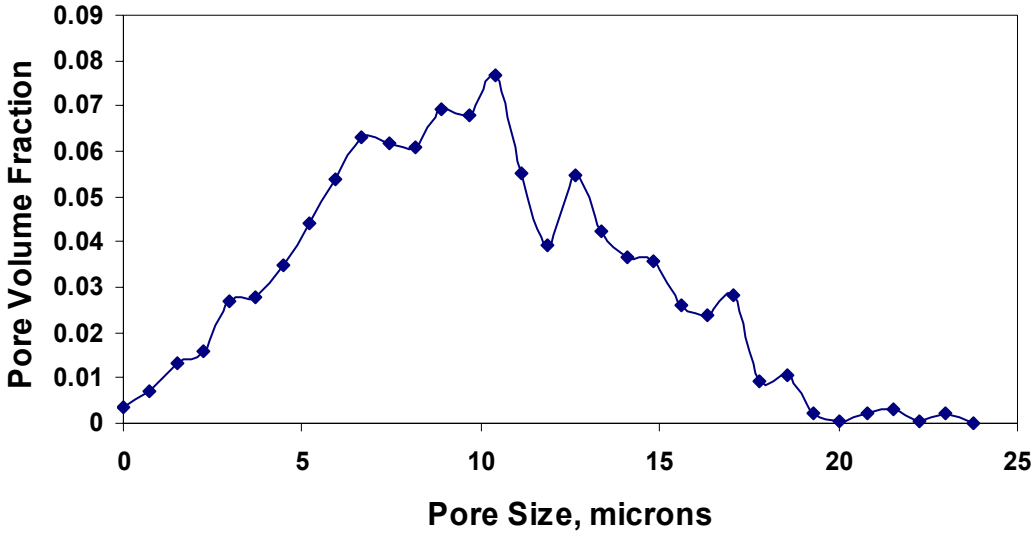

**Fiber shape and structure measurements for Lattice Boltzmann Model microstructures**



**Zoomed view to look in the pore**

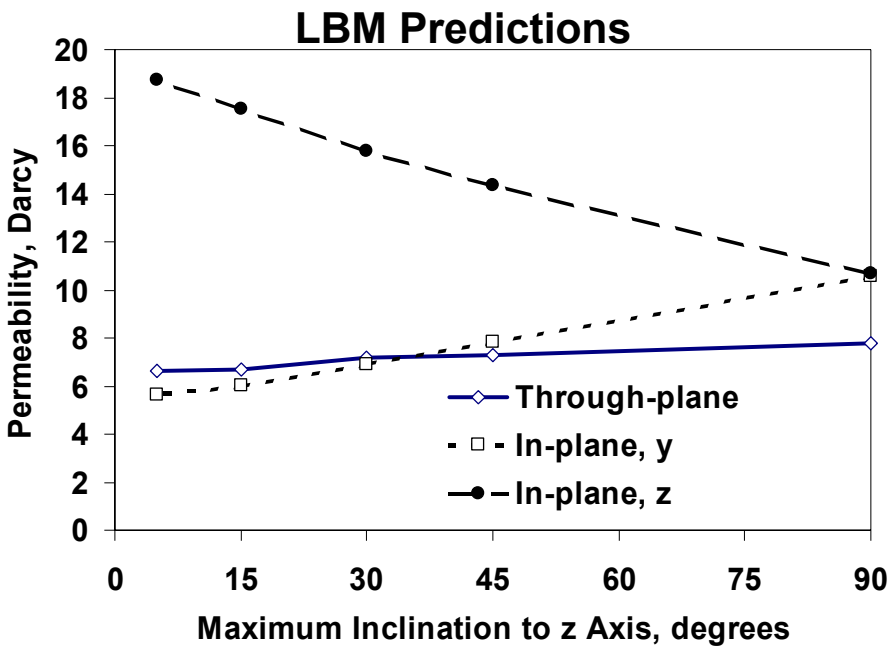
# GDL Microstructure Generation

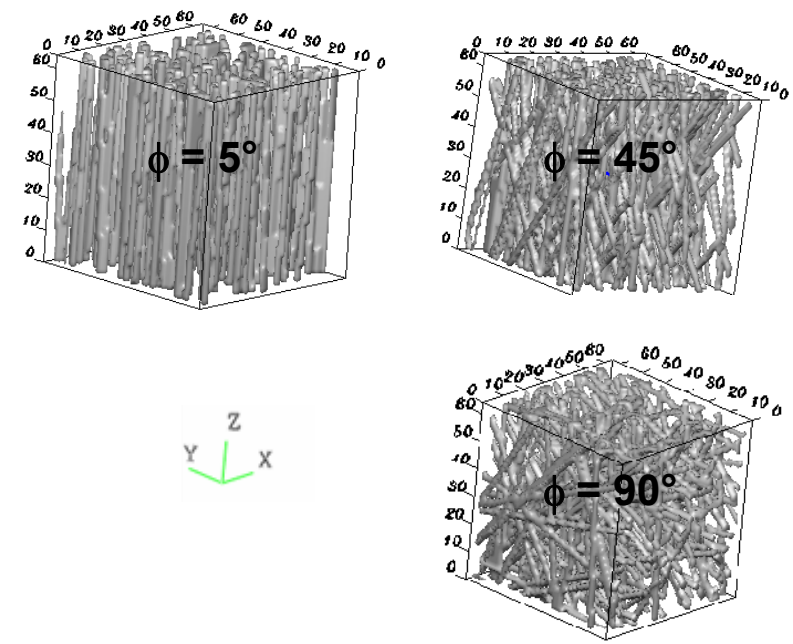



- **Porous Microstructure:**
  - **Need to adequately capture distribution of fibers and PTFE on fiber mesh, fiber shape, overlapping fibers.**
- **Status:**
  - **Generating from stochastic distribution of fibers**
  - **Computing pore size distribution to evaluate model consistency with actual structure**
- **Ongoing Development:**
  - **Non-uniform Teflon distribution**
  - **Addressing fiber shapes (crimped, bent), response to clamping pressure.**

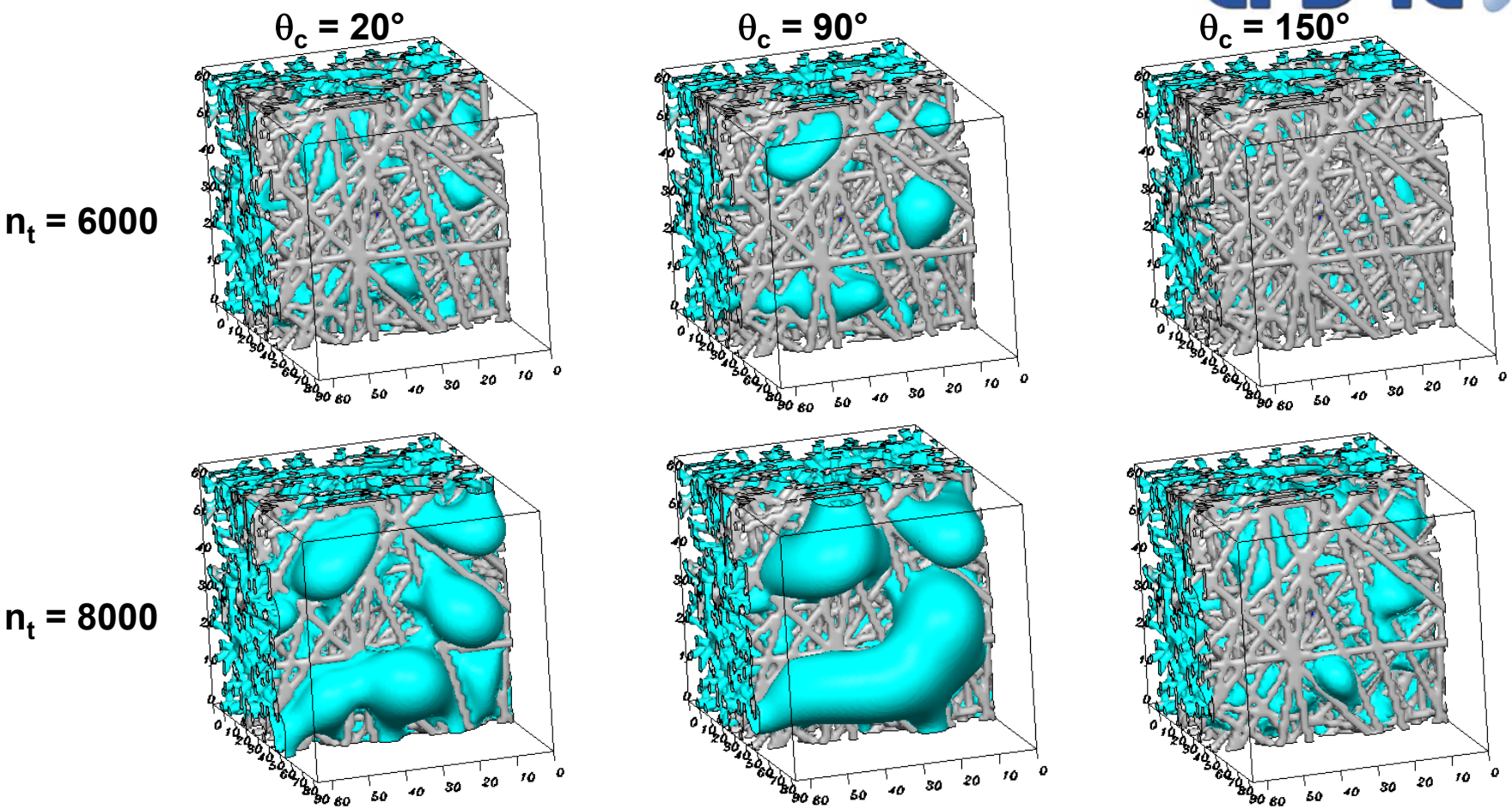
# GDL Properties vs. Microstructure




- Implemented single-phase Lattice-Boltzmann (LB) model, validated against canonical problems including flow through pores in regular sphere packs. Permeability computations for reconstructed GDLs are consistent with published data
- Applied to single-phase permeability simulation for non-woven GDL structures with varying degrees of fiber alignment
- Control of in-plane:through-plane permeability ratio demonstrated as feasible, potentially valuable for water management

# GDL Treatment and Water Transport




- Implemented isothermal, immiscible, two-phase LB model including surface wettability effects and validated by canonical test cases of drop equilibration.
- Transient simulations of liquid water transport into 200 μm thick GDL materials show preferred emergence locations, consistent with experimental observations
- Emergence locations are independent of fiber surface treatment (uniform equilibrium contact angle for all fiber surfaces)

# Future Work and Milestones

**FY08-09 Plans:**

- **Characterization and Diagnostics**
  - Complete first round of ex-situ characterization studies (GDL microstructure, transport properties, freezing point); GDL-channel transport experiments
  - Component interaction and flooding sensitivity studies in S-H cells
- **Model Development/Testing**
  - Apply and assess LBM for two-phase transport property prediction
  - Complete GDL Transport and GDL/Channel interface model implementation in cell-scale models, address freeze-thaw phase change
  - Water management improvement concept(s) development and screening

**Upcoming Milestones and Decision Points:**

- LBM: continued development and/or application decision
- Cell Scale model evaluation against ex-situ validation data (water and gas two-phase transport in GDL, GDL+channel), and steady-state diagnostic data

# 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:**
  - Characterized key physical and transport properties for SGL GDL materials, initial microstructure analysis of Ballard materials
  - Demonstrated self-humidified cell diagnosis by IR, gathering performance data and diagnostics for effects of materials and operating conditions
  - LBM developed and validated for single-phase and two-phase flow with porous media; applied to analyze microstructure impact on permeability, common liquid breakthrough pattern observations
  - Evaluated initial cell scale model capabilities and needs for 2-phase transport in GDL, began implementation and tests
- **Proposed Future Work:**
  - Continue evaluating and improving characterization, diagnostics, and models; apply validated measurements and simulation tools to identifying optimization strategies