Better Decisions, Better Products Through Simulation & Innovation

DOE Hydrogen Program

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

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CFDRC

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Project ID: 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

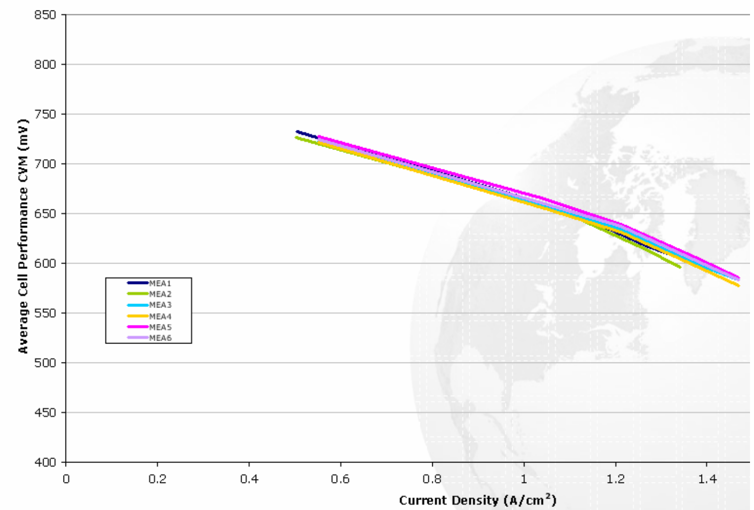
- **Barriers:**
  - D. Water Transport within Stack
  - E. System Thermal and Water Management
  - G. Start-up and Shut-down Time and Energy / Transient Operation

- **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)

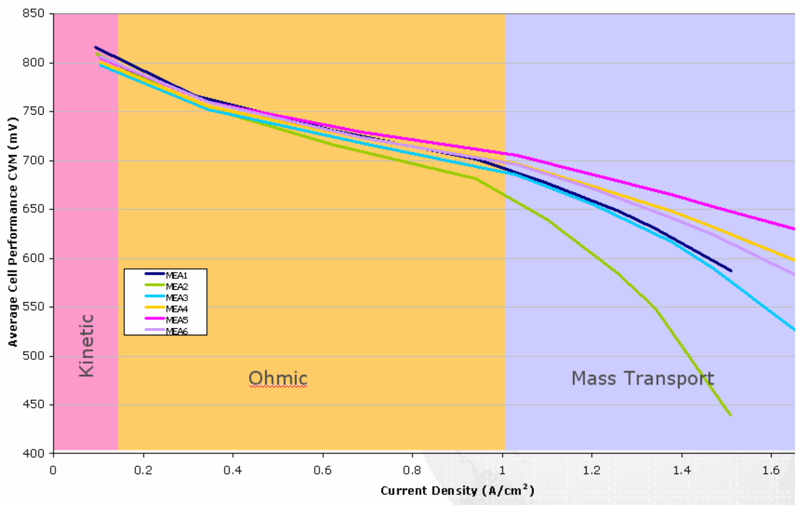
- **Partners:**
  - Ballard Power Systems
  - BCS Fuel Cells
  - ESI Group, NA
  - Research Triangle Institute
  - SGL Carbon
  - U. Victoria

Water Management & Performance

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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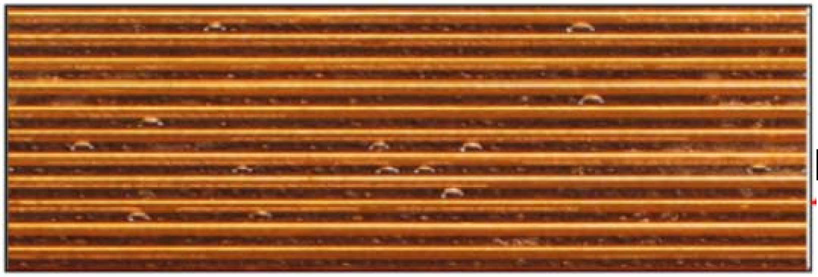
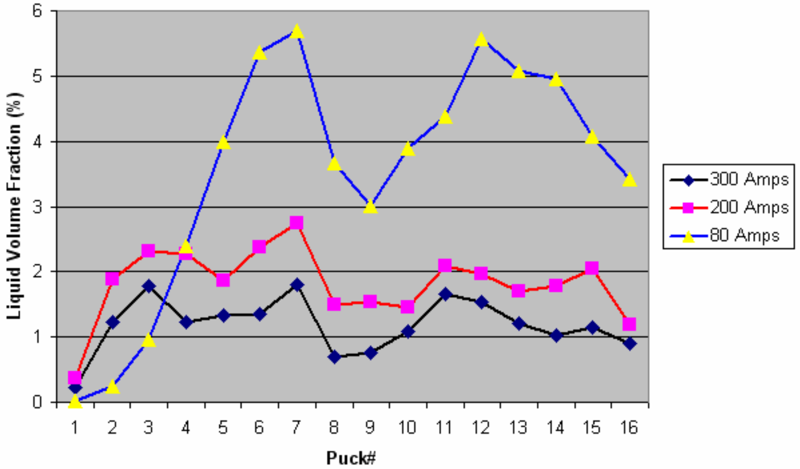
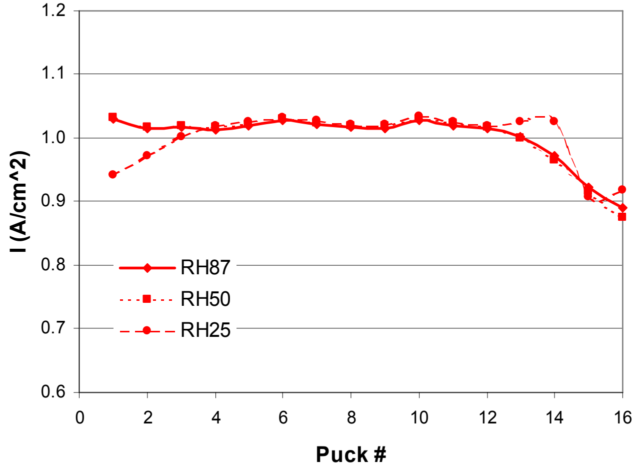
FlowViz for liquid water measurement in channels of an operating cell



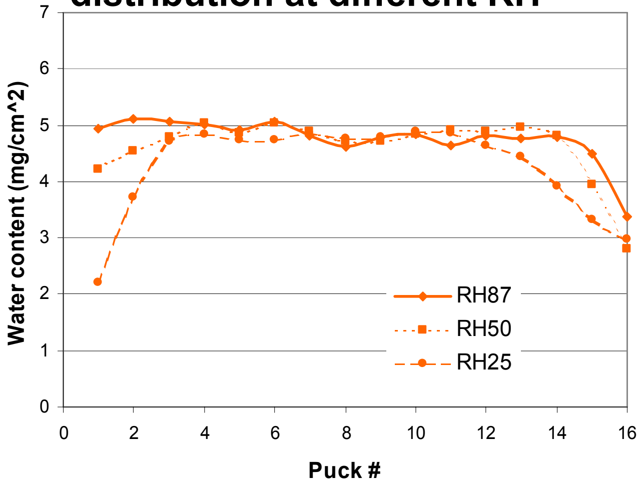
Measured liquid water volume fractions in channels at 16 pucks along the cell



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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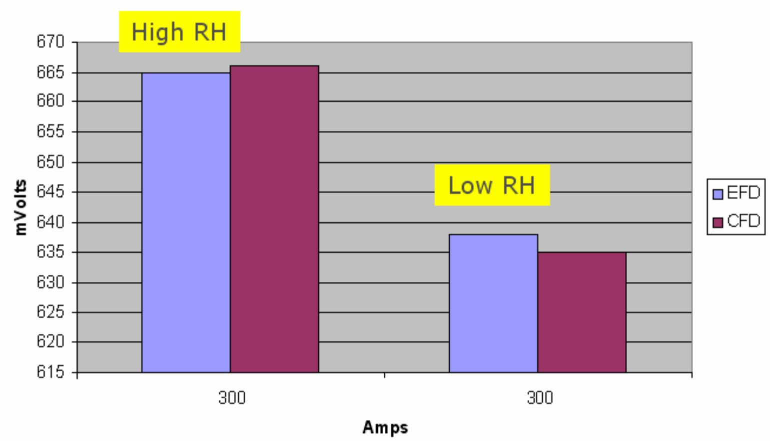
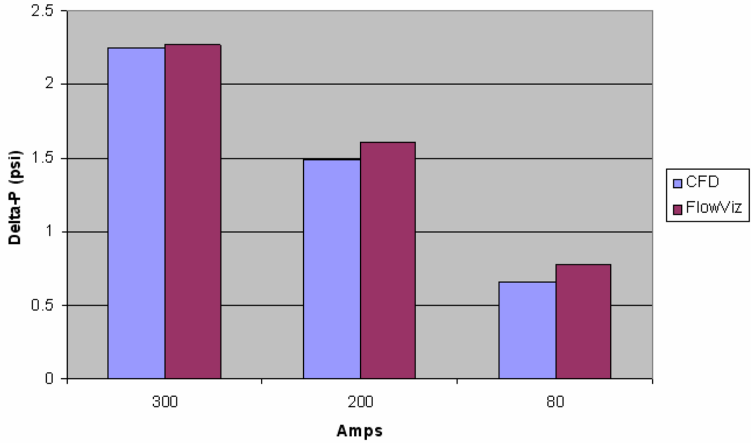
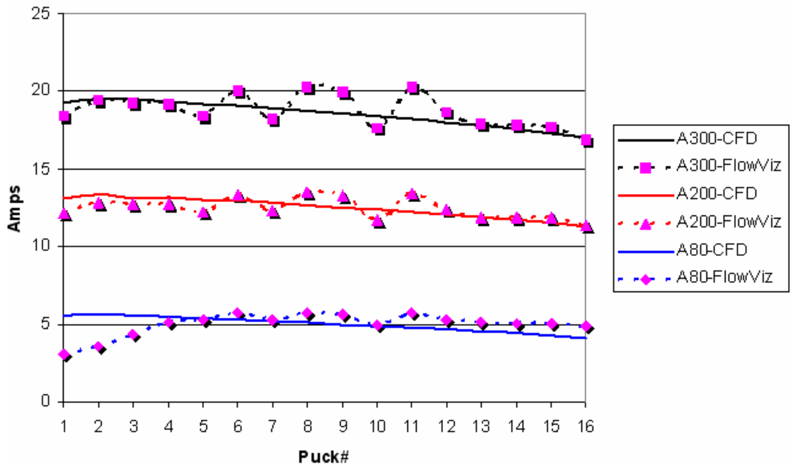
Measured vs Predicted cell performance at different RH



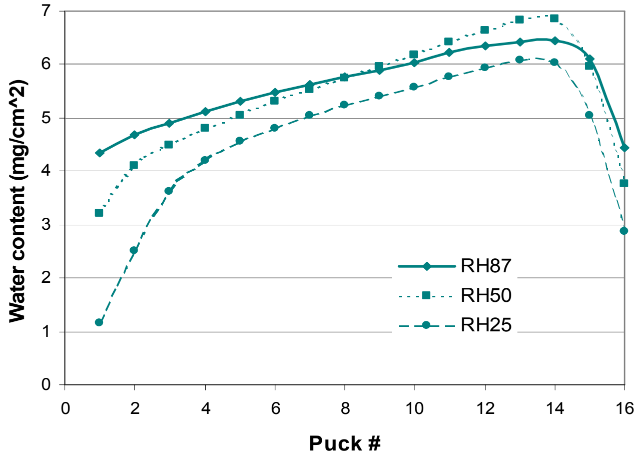
Measured vs Predicted wet pressure drop in cell at different currents



Measured vs Predicted current distributions



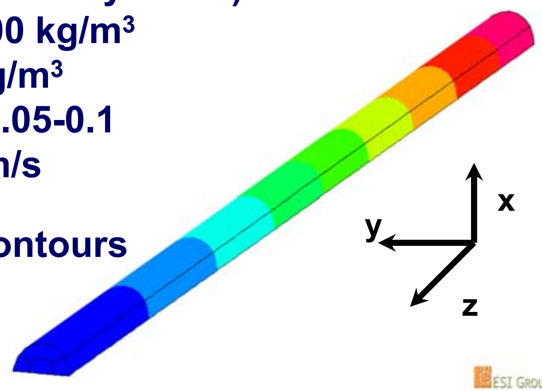
Predicted MEA water at different RH



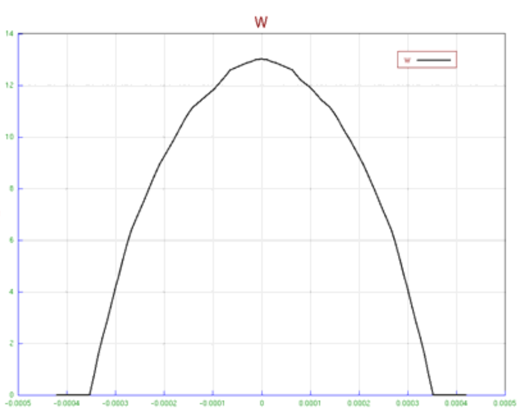
Cell Scale Model Improvements

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

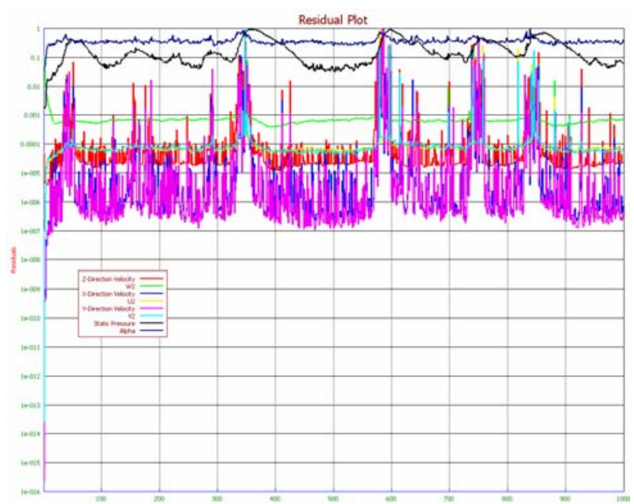
Pressure Contours



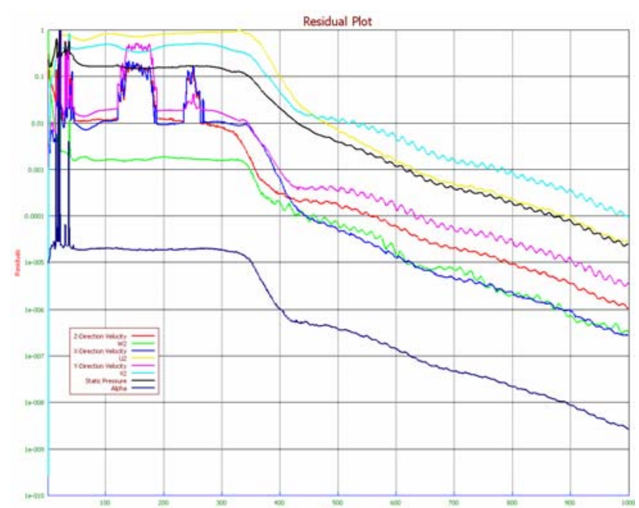
- Selected true two-phase flow treatment as transport formulation
- Extended two-phase flow to address porous media
- Improved convergence and robustness for two-phase flow analysis of channels



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



Formulation (A)

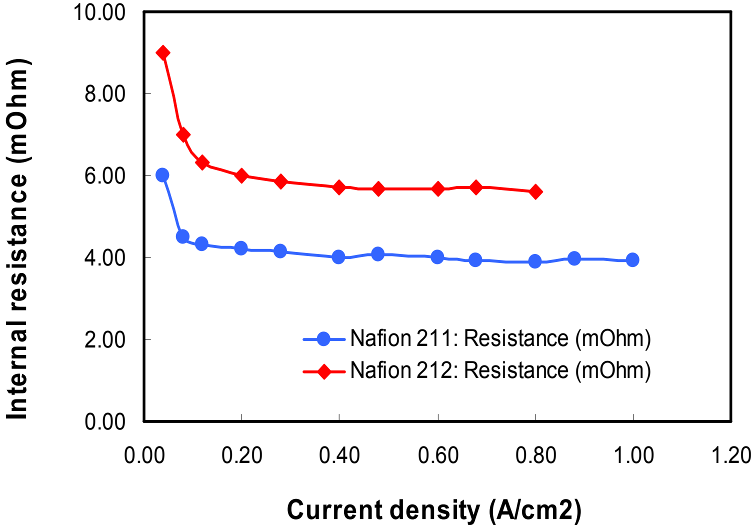


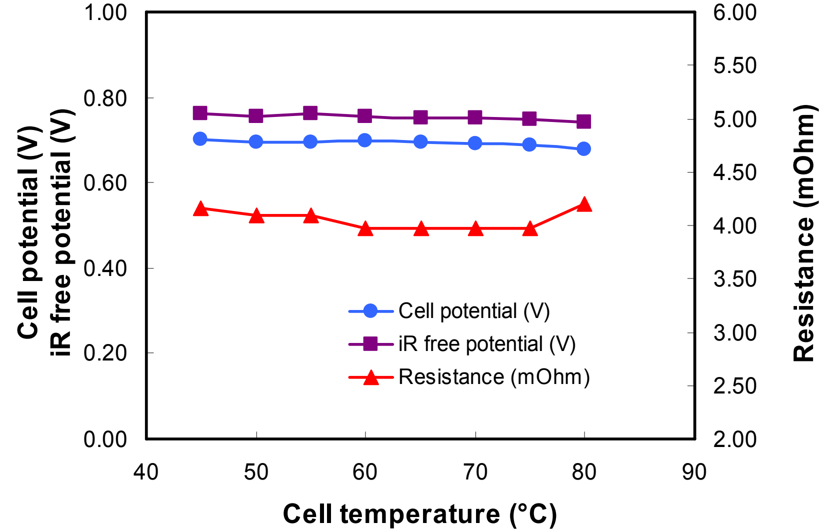
Formulation (B)

Convergence Plots

Self-Humidified Cell Diagnostics

BCS Fuel Cells, Inc

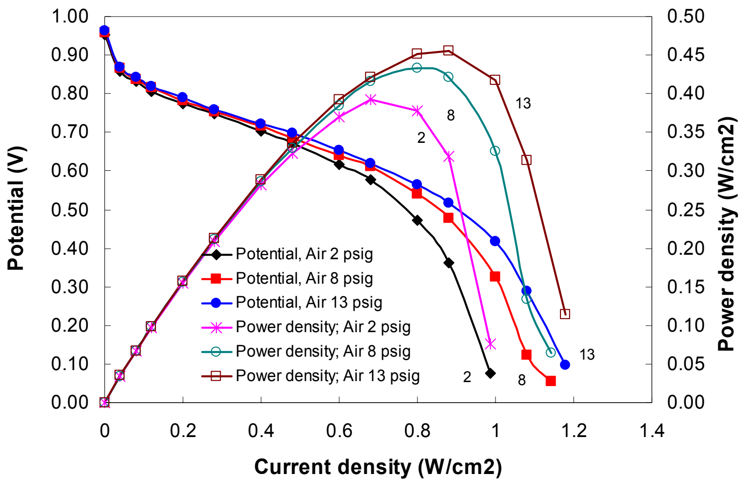


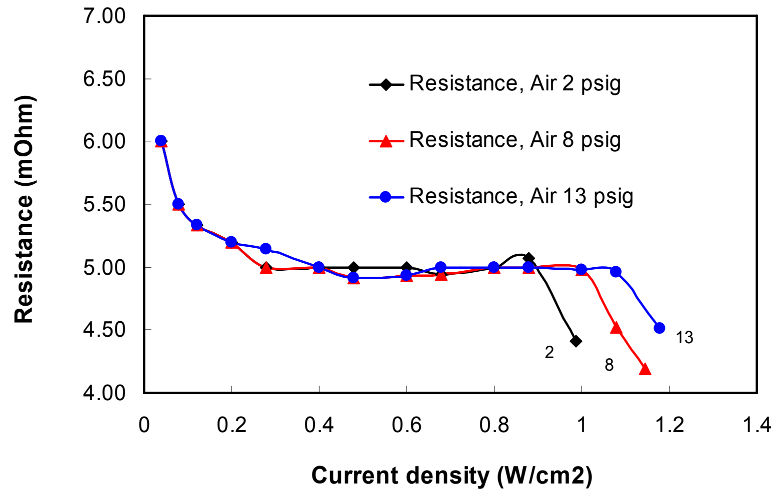


- **Established current interruption based Internal Resistance, IR, drop measurement technique in single cells**
  - **Measured IR with membranes Nafion 211 and 212, the expected distinct differences in cell resistance are observed**
  - **Single cell IR using Nafion 211 membrane drops with increasing 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:

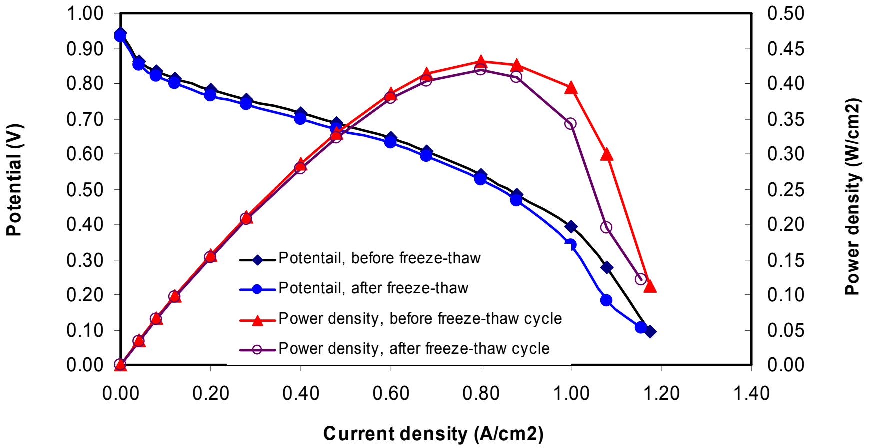
Air stoic: 1.25; Temp: 40 °C; H2 pressure: 2 psig, Anode 0.2 mg/cm^2 Pt, Cathode 0.5 mg/cm^2 Pt

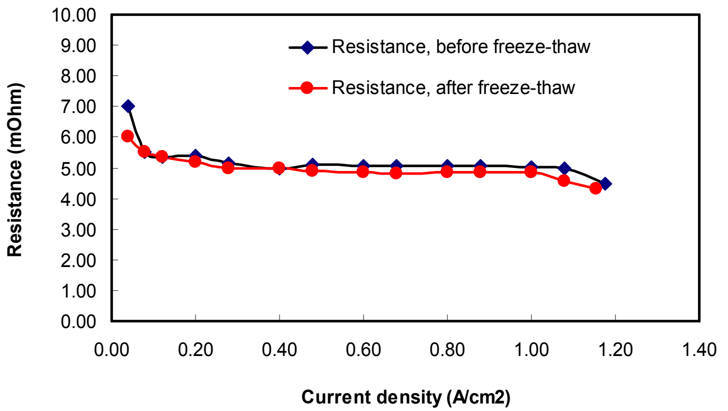
- **Established detection of accelerated electrode flooding using GDL with low Teflon content, 5%, in the micro-porous layer (MPL)**
  - **Plot shows V-I and W-I data extending to extreme mass transfer control (EMTC) regime**
  - **A sudden or sometime a gradual drop in IR in the EMTC region is indicative 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



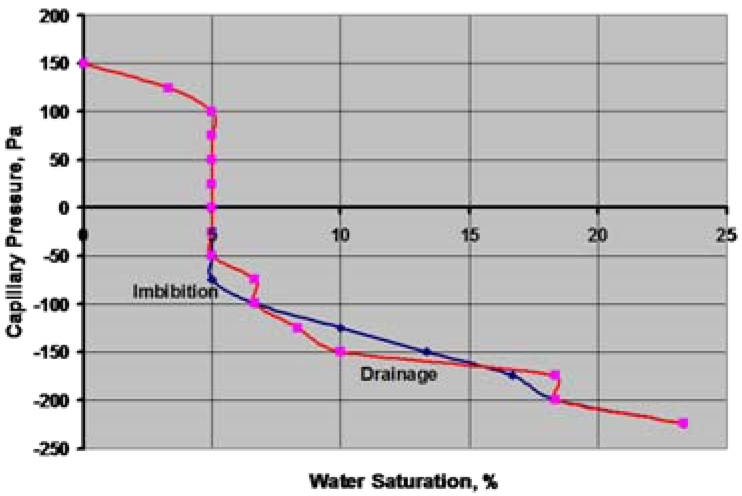


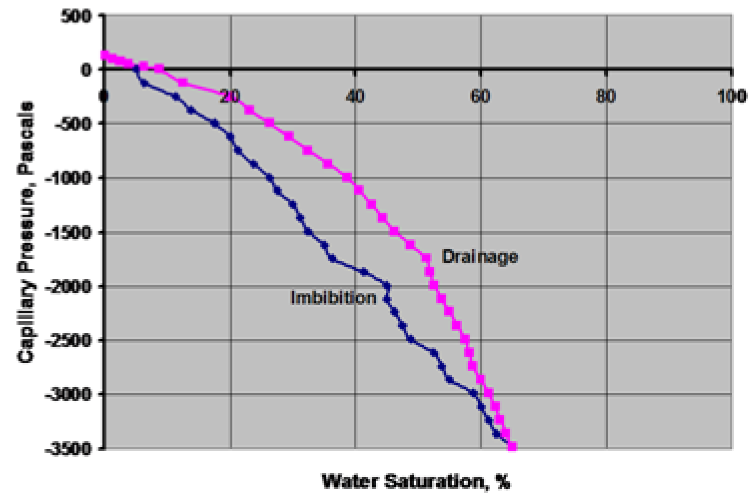
- **Initiated Freeze-Thaw Cycle (F-TC) tests in single cells to study the effect on performance and electrode flooding behavior. Cell frozen to -20°C, 6 cycles**
- **Cell performance slightly drops with F-TC, internal resistance drop at high currents indicates electrode flooding before and after cycling**
- **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

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

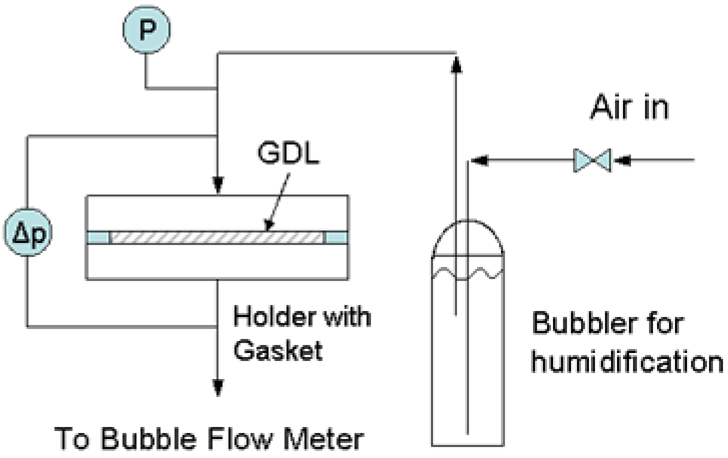
- **Positive Water Displacement technique**
  - **90 mm diameter media for greater resolution in water uptake measurements**
- **Water breakthrough observed at isolated locations on GDL surface limiting water saturation of media**
- **Characterizing SGL provided materials**
  - **Series 24, 25, 34, and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





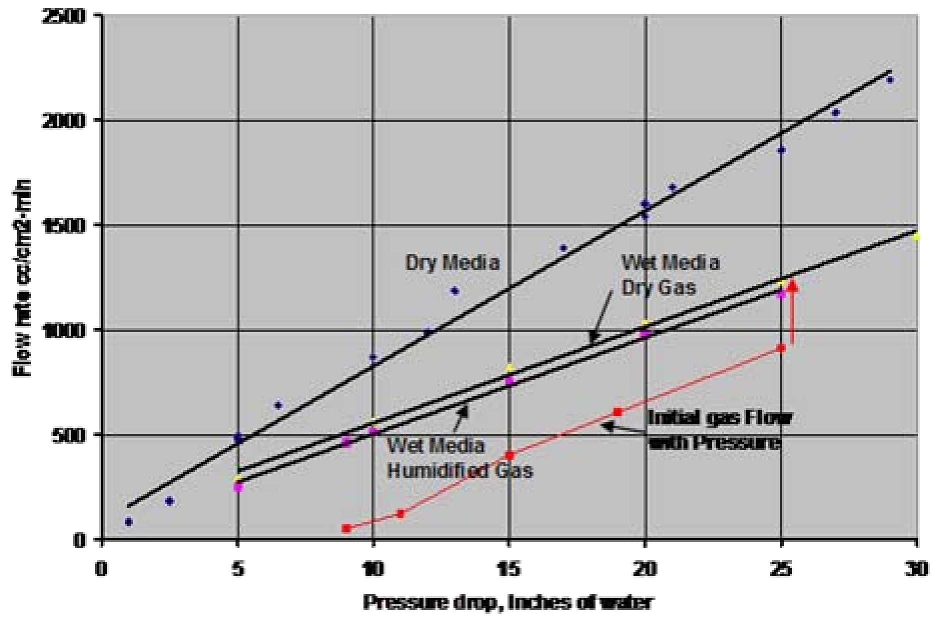
- **SGL 24 BC – 218 µm:**
  - **Coarser pore size, thinner media**
  - **No hysterisis behavior**
  - **Quick breakthrough at low ΔP**
- **SGL 35 BC – 321 µm:**
  - **Finer pore size thicker media**
  - **Hysterisis in imbibition/drainage**
  - **Need high ΔP for breakthrough**

Gas Permeability of Dry/Wet GDL



Permeability Flow Apparatus

SGL 35BC Wet Permeability Characterization



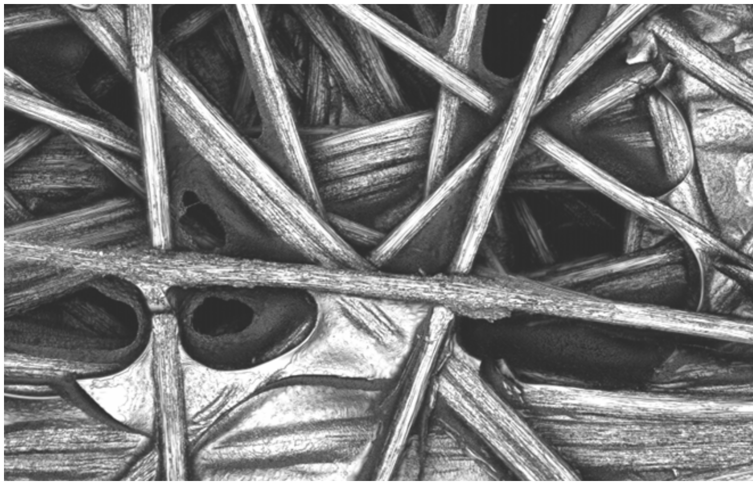
- **Dry permeability with dry GDL**
- **For wet permeability GDL is initially filled with water under pressure, gas flow used to expel part of the water (red curve in figure)**

- **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**

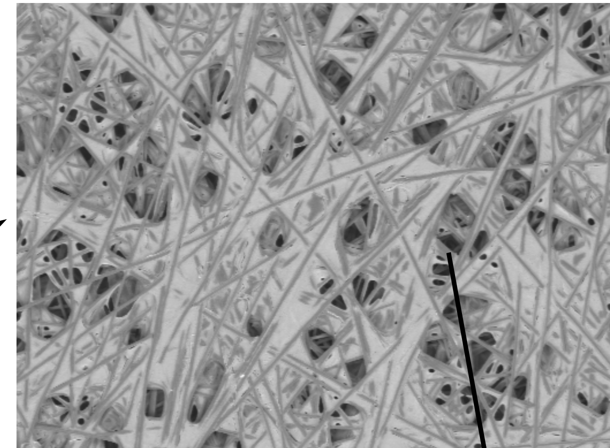
GDL Microstructure Characterization

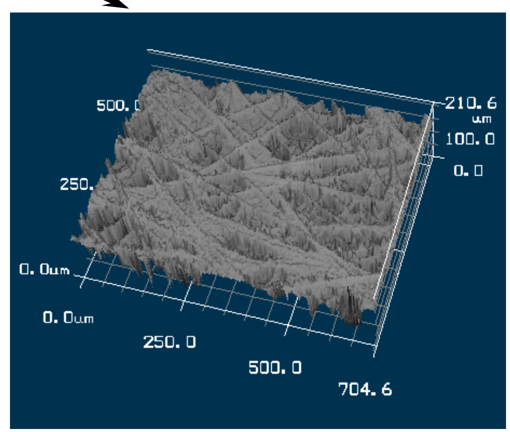
BALLARD

Laser Microscope imaging of a teflonated GDL for structure

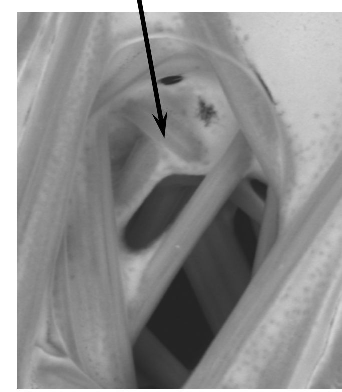


SEM imaging to identify teflon



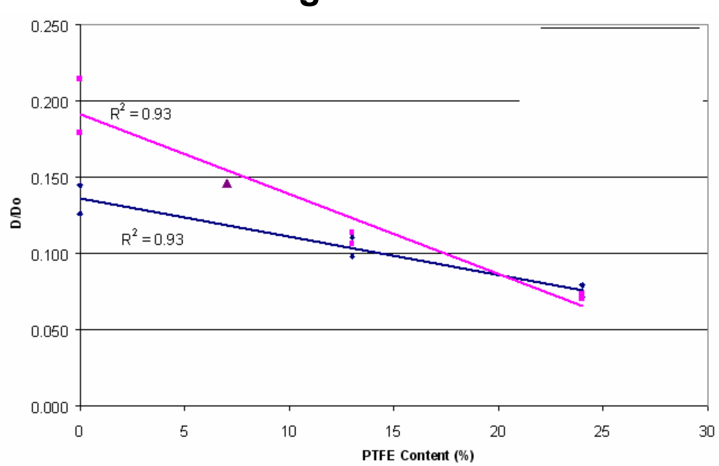


Fiber shape and structure measurements for Lattice Boltzmann Model microstructures

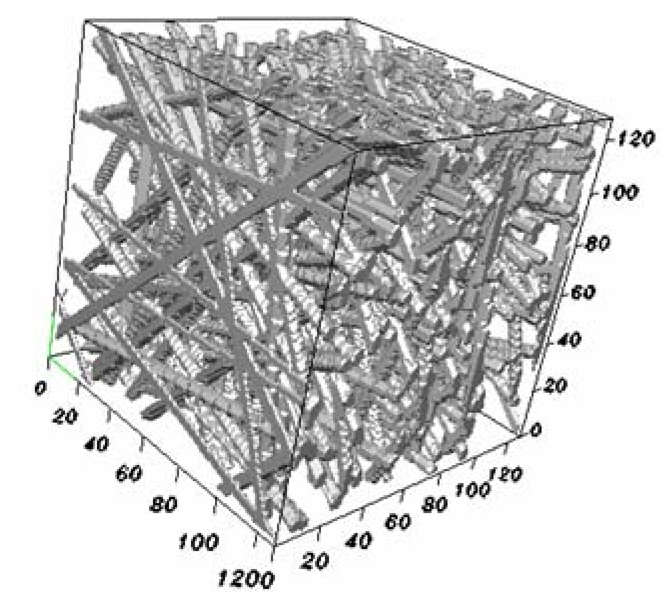


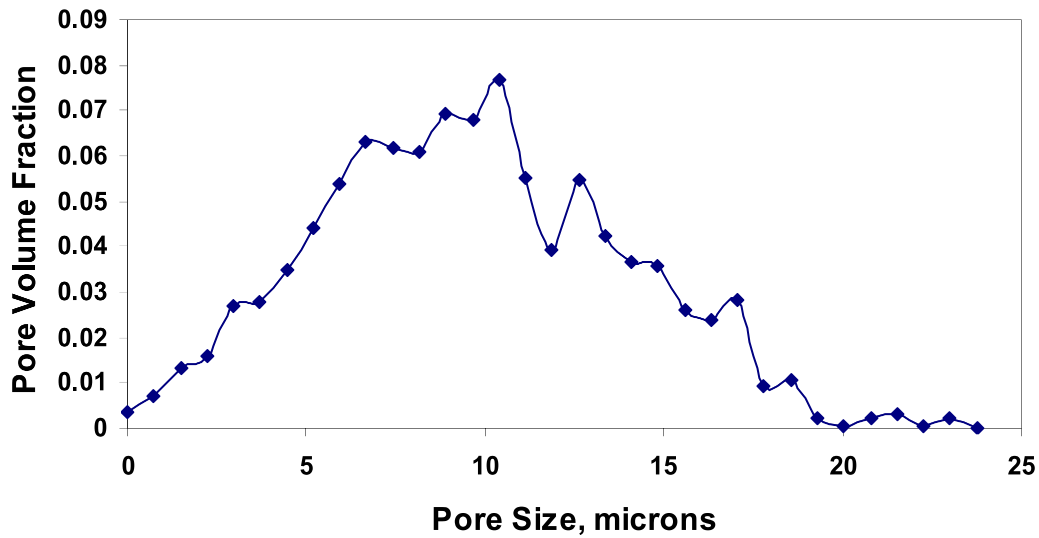
Zoomed view to look in the pore

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



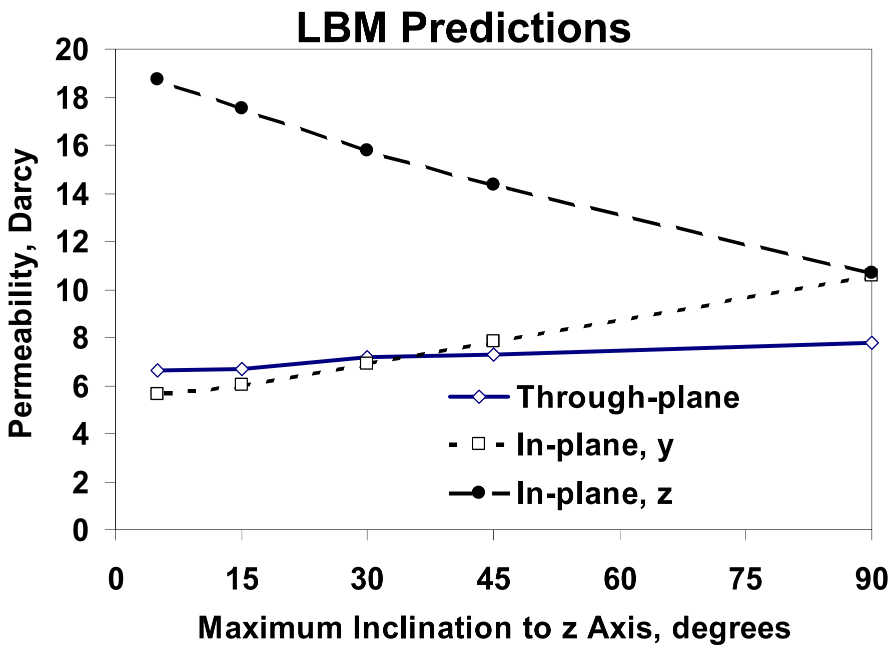
GDL Microstructure Generation

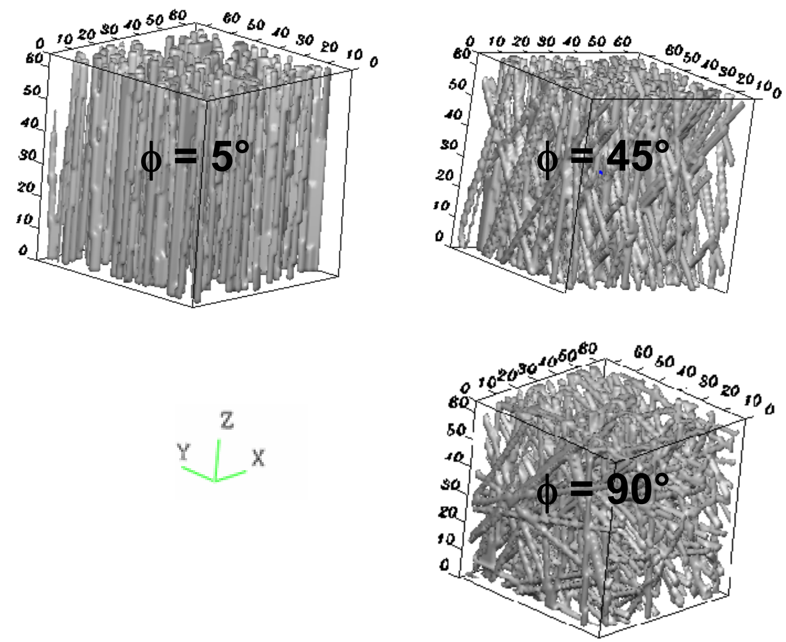




- **Porous Microstructure:**
  - **Need to adequately capture distribution of fibers and PTFE on fiber mesh, fiber shape, overlapping fibers.**
- **Status:**
  - **Generating from stochastic distribution of fibers**
  - **Computing pore size distribution to evaluate model consistency with actual structure**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

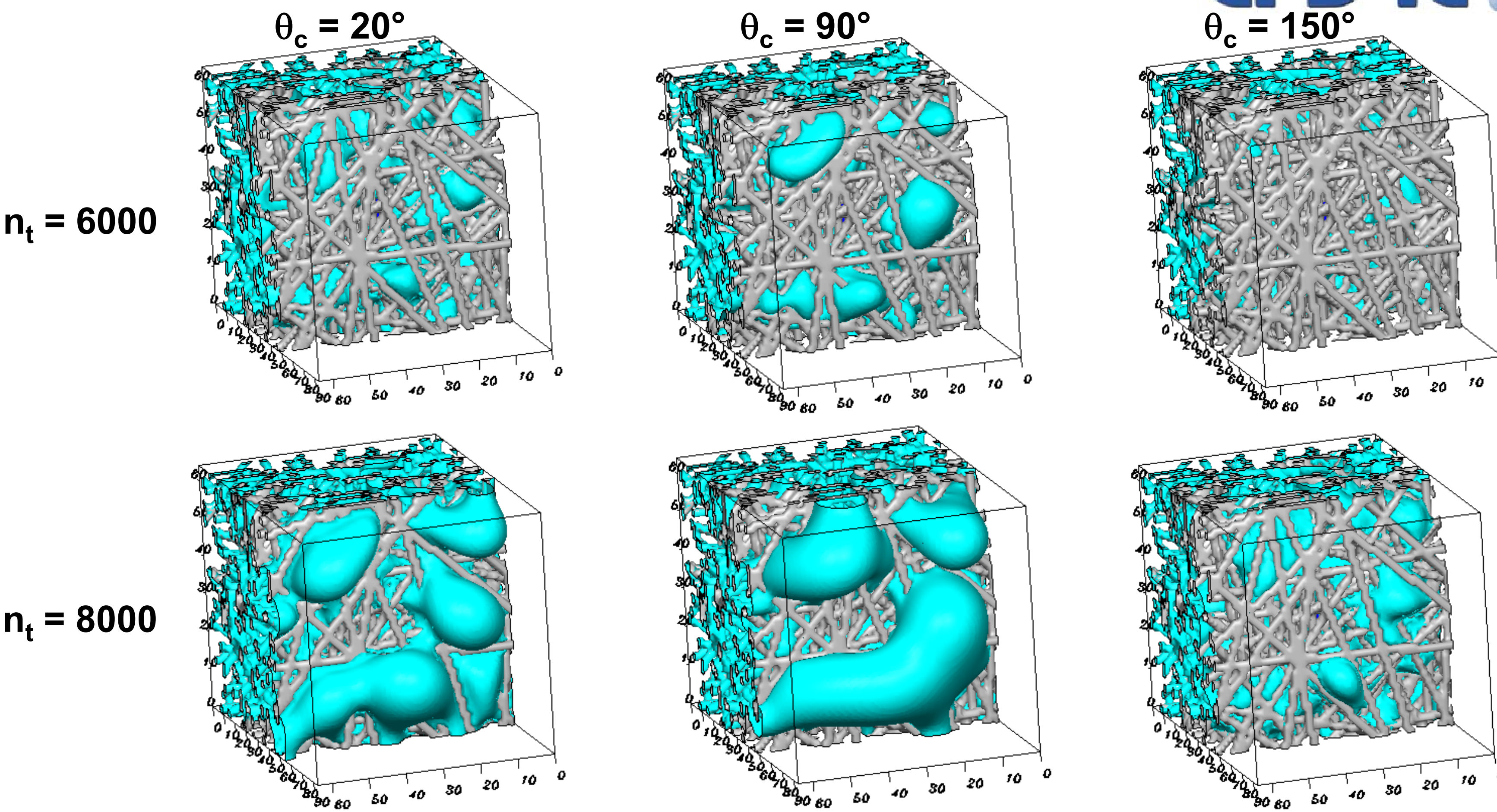
GDL Properties vs. Microstructure





- 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**