CFDRC • • • Delivering Breakthrough Solutions

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

J. Vernon Cole

CFD Research Corporation

May 15, 2012

Project ID: FC030

Overview

- **Timeline**
  - **Start Date: 6/1/07**
  - **End Date: 5/31/12**
  - **Percent Complete: 95%**
- **Budget:**
  - **Total Project Funding:**
    - **DOE share $ 4,958K**
    - **Cost share $ 1,464K**
  - **Funding Received in FY11: $ 818K**
  - **Planned Funding for FY12: $ 0**
- **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

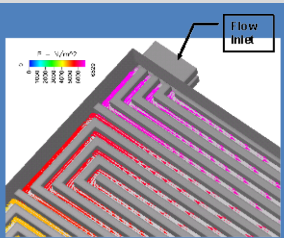
- **Overall:**
  - **Improve understanding of the effect of various cell component properties and structure on the gas and water transport in a PEM fuel cell;**
  - **Demonstrate improvements in water management in cells and short stacks; and**
  - **Encapsulate the developed understanding in models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

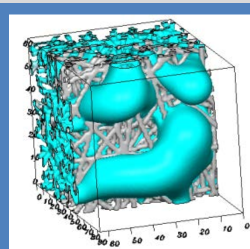
- **FY 2011 and 2012:**
  - **Complete cell scale model testing and validation against steady state and transient operational cell data**
  - **Complete fuel cell water transport model improvements and code package development to include two phase flow**
  - **Complete validation of water transport model based on data gathered during optimization studies, and make recommendations for water management improvement including operating strategies and GDL materials modification.**
    - **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**

Approach

Improved Water Management Through Improved Component Designs and Operating Strategies

Advanced Model Development (CFD/Lattice Boltzmann Method)

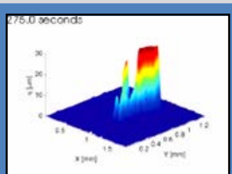


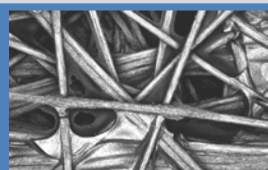


- LBM models for microscale flow thorough porous media: in-plane and through-plane permeabilities, capillary pressure, and wetting characteristics
- CFD models for macroscopic two-phase flow in channels, GDLs and interfaces, coupled with electrochemical reaction and transport through membrane

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

Experimental Characterization



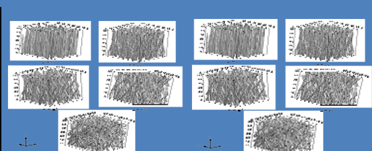


- Ex-situ characterization: key materials properties and sensitivity to treatments, water transport analysis in GDLs and micro-channels
- In-situ diagnostics: current and water distribution

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

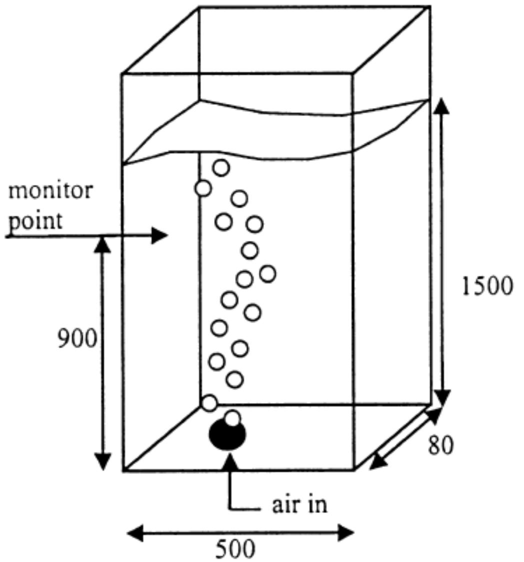
Improved component designs and operating strategies, tools for addressing water transport in future generation designs

FY 11-12 Plans and Milestones

Month/Year	Milestone	Comments	% Complete
Mar 12	Cell scale models tested and validated against steady and transient operational cell data	Steady state results show less mass transfer effect than expected; additional transients needed	90%
Mar 12	Complete fuel cell water transport model improvements and code package development	Source code transferred to ESI, user interfaces complete; test battery of sample models to be executed	90%
May 12	Complete validation of water transport model and make recommendations for water management improvement	Two-phase flow, porous media without capillary pressure complete and model formulation improved	80%

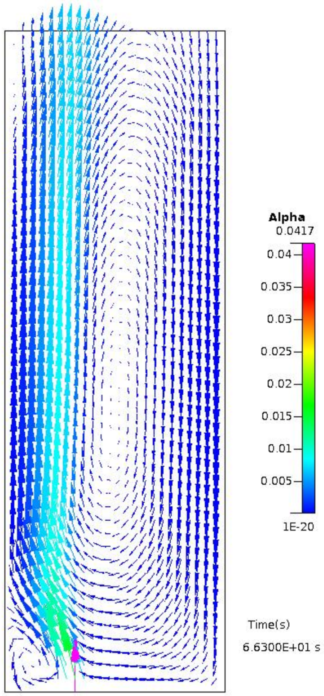
Recent Accomplishments: Model Evaluation: Two-Phase Flow Benchmarks

Bubble Column Experimental Setup



- Air injected at bottom, 1.6 l/min
- Water velocity sampled at the monitor point

CFDRC/ESI Results and Benchmark†



ESI Result

Mudde et al. benchmark results:

- Steady 0.144 m/s vertical velocity at the monitor point after 40 seconds
- Slightly more gas dispersion, due to symmetry condition instead of outlet at the top

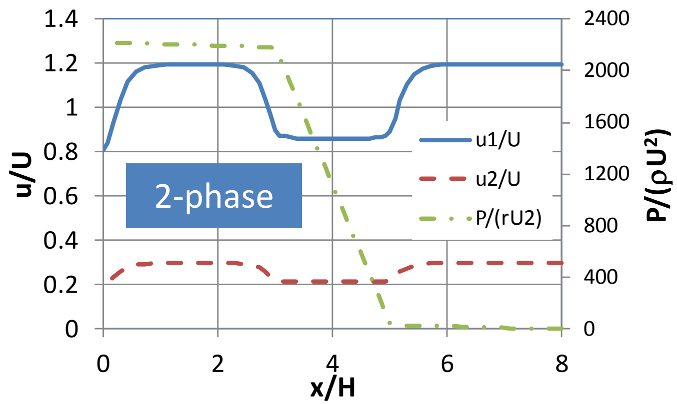
▪ Good agreement for gas fraction distribution, time scale (45 seconds to steady state) and steady velocity at the monitor point (0.142 m/sec) in 2-dimensional test model

† R. F. Mudde, O. Simonin, 1999, " Two and three-dimensional simulations of a bubble plume using a two-fluid model.", Chemical Engineering Science 54 (5061)

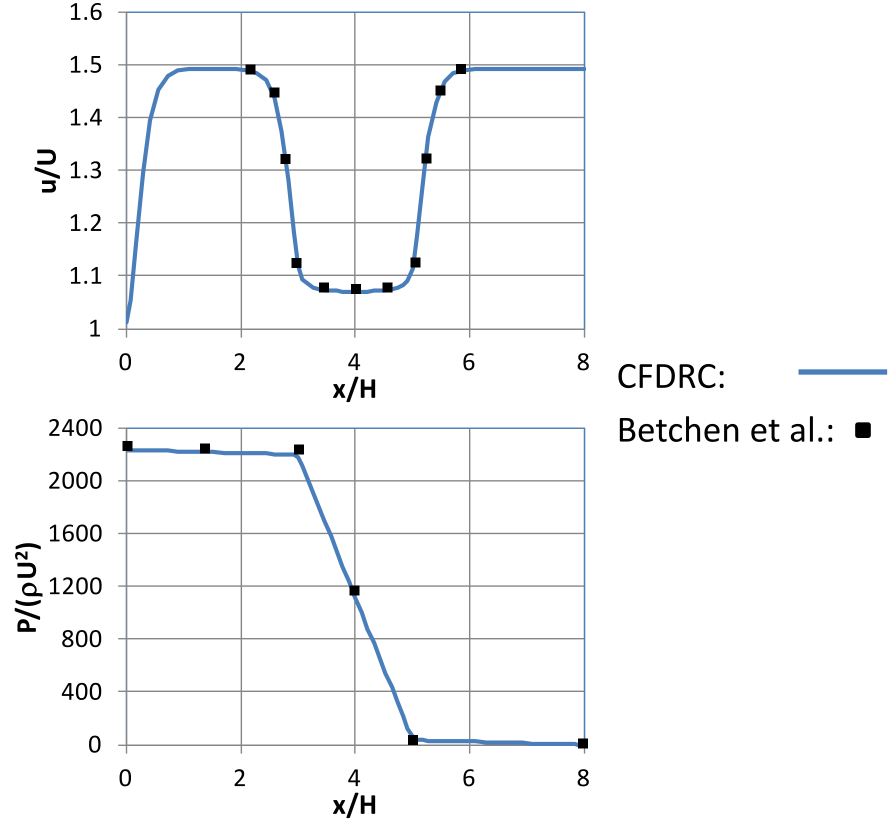
Recent Accomplishments: Model Evaluation: Porous Media Flow Benchmarks

Porous Plug Test Case

- Channel with porous plug, plug length = 3H
- Darcy and Forcheimer drag terms included
- Re=1, ε=0.7, Da=10^{-3}



CFDRC/ESI Results and Benchmark†

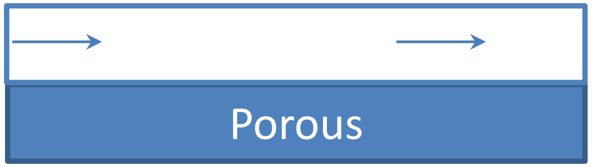


- Boundary treatment at open/porous interfaces improved to avoid pressure or velocity discontinuities; two-phase for identical fluids (ρ, μ) α=0.2

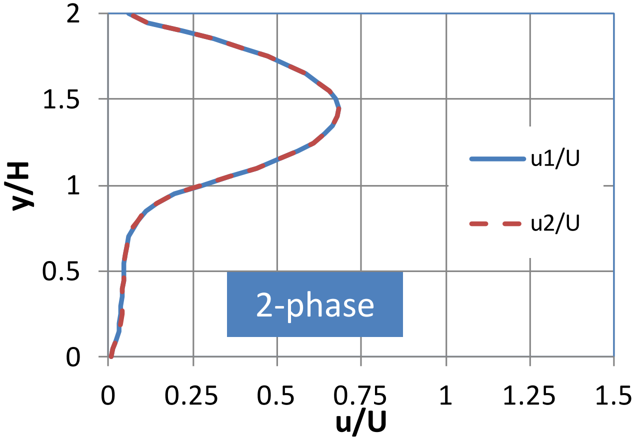
† Betchen, L., et al. "A Nonequilibrium Finite-Volume Model for Conjugate Fluid/Porous/Solid Domains," Numerical Heat Transfer: Part A: Applications 49, 543-565 (2006).

Recent Accomplishments: Model Evaluation: Porous Media Flow Benchmarks

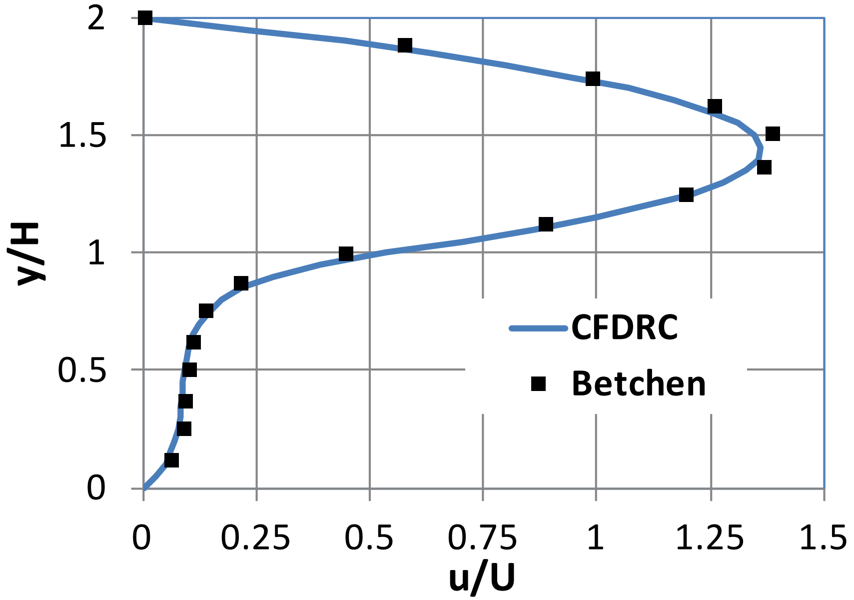
Beavers-Joseph Problem



- Channel with porous region
- Re=1, ε=0.7, Da=10^{-2}



CFDRC/ESI Results and Benchmark†

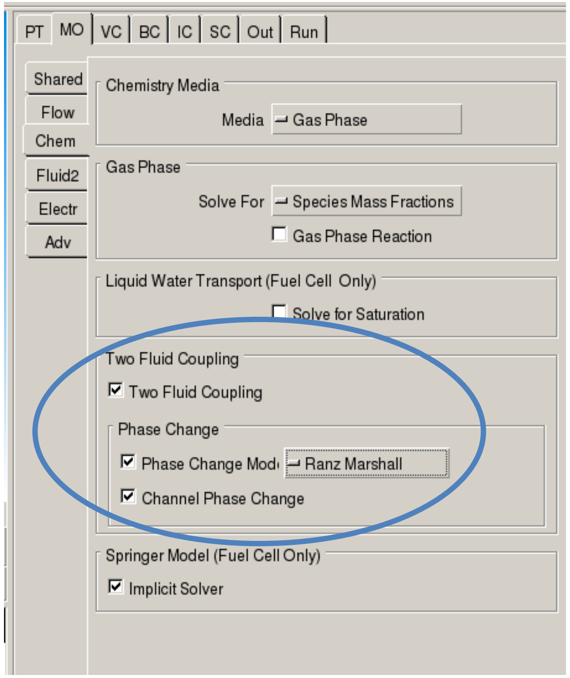


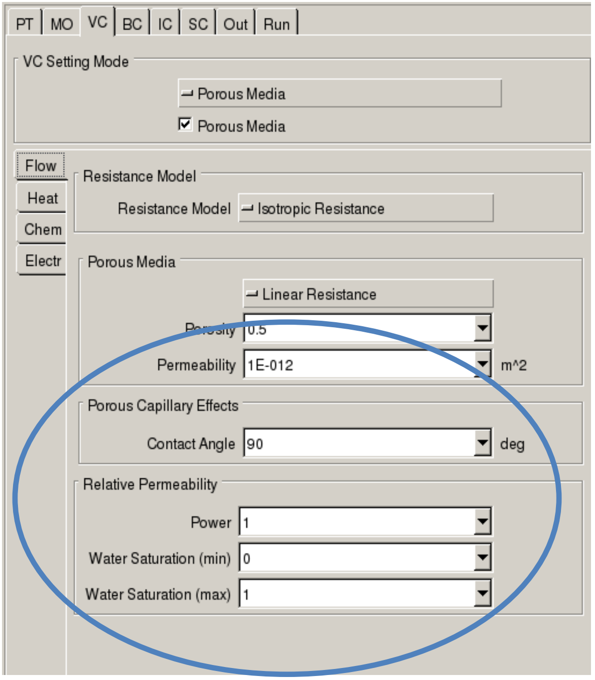
- Good agreement at open/porous interfaces; no pressure or velocity discontinuities; two-phase results for identical fluids (ρ, μ) α=0.5

† Betchen, L., et al. "A Nonequilibrium Finite-Volume Model for Conjugate Fluid/Porous/Solid Domains," Numerical Heat Transfer: Part A: Applications 49, 543-565 (2006).

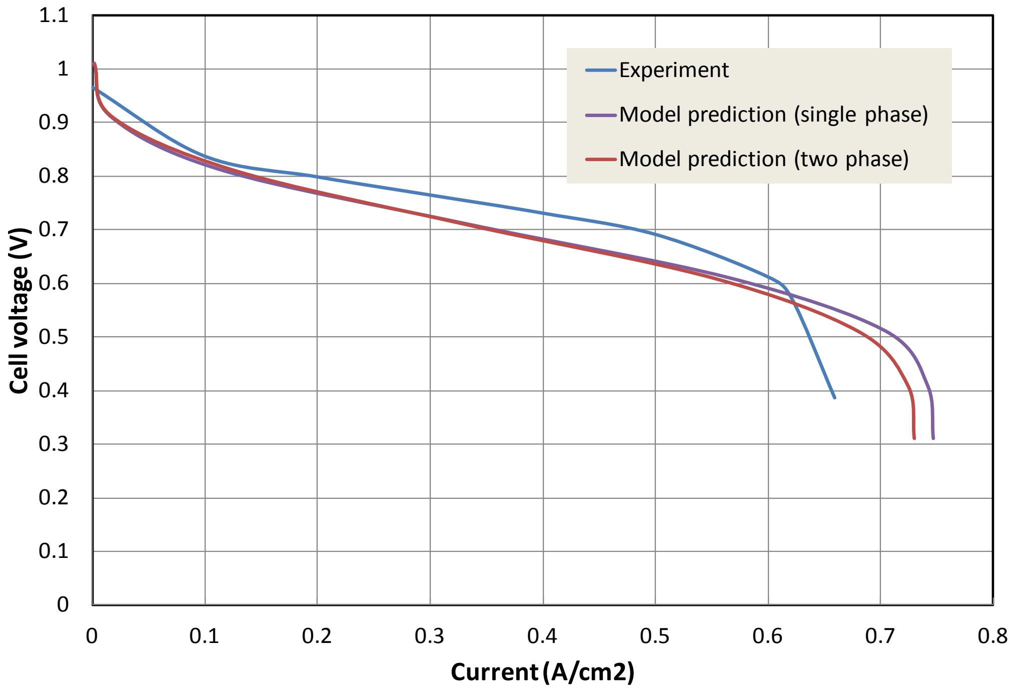
Recent Accomplishments: Software Package Development

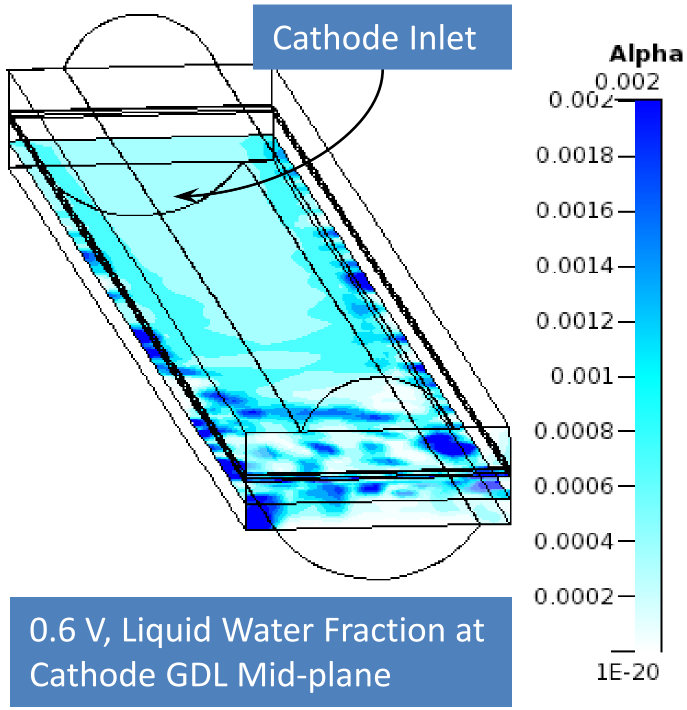
- ESI has integrated the developed models into the commercial version of CFD-ACE+
- GUI development to allow water transport model options and parameters complete





Recent Accomplishments: Model Evaluation: Operational Cell

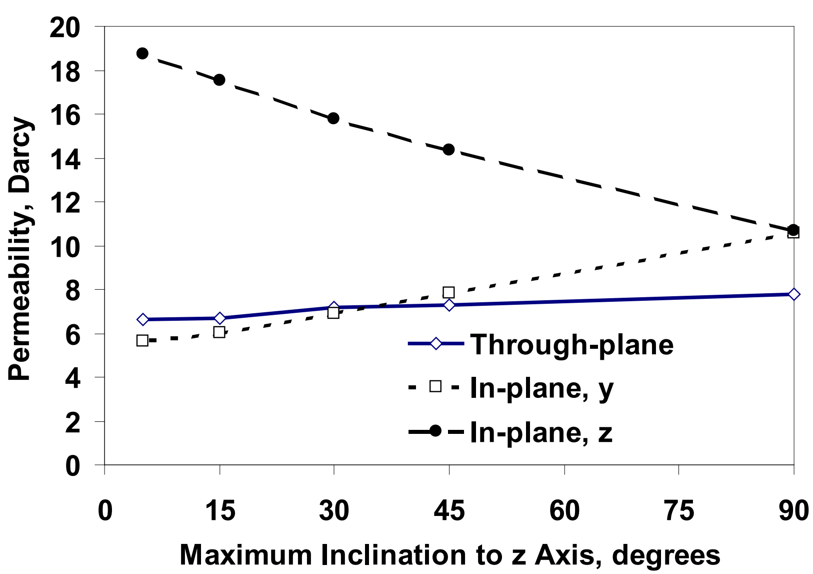


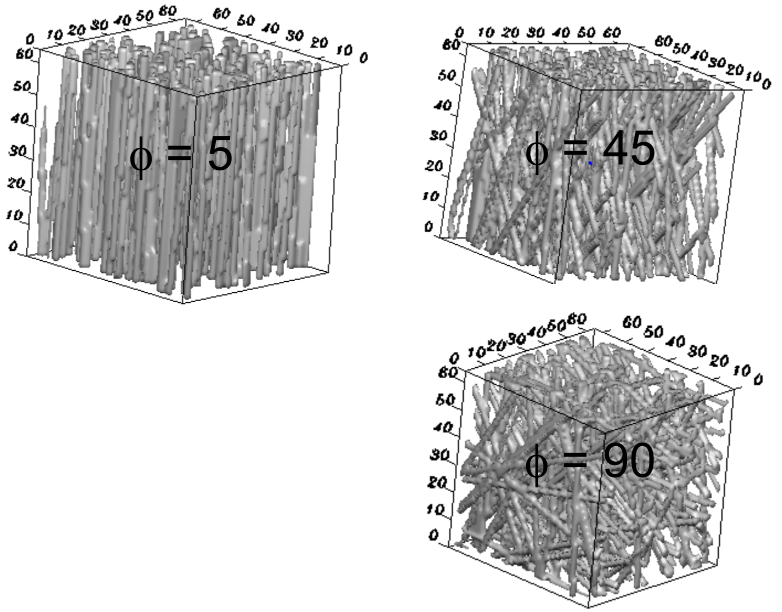


- Testing against characterization data gathered by Ballard in a test fixture operating at high stoichiometry:
  - 60 °C and 100% relative humidity operation
  - Based on measured effective diffusivity, transport limitations at 0.6 A/cm^2 should be due to only liquid water presence in GDLs and catalyst layers, $\alpha \approx 0.1$ needed with typical water effect on effective diffusivity

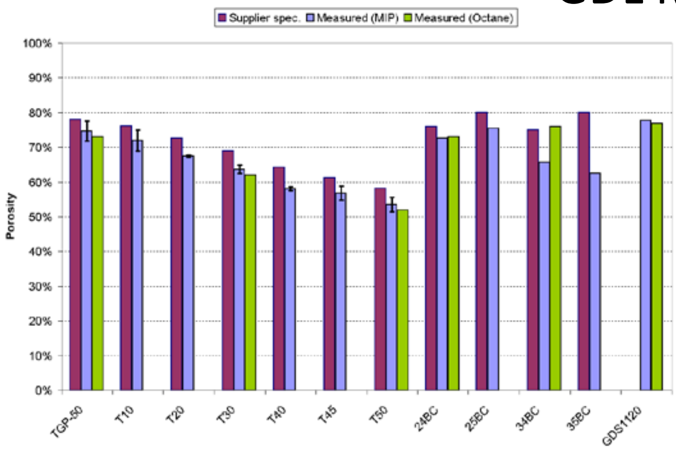
Overall Accomplishments: Materials Concept Screening (2008)

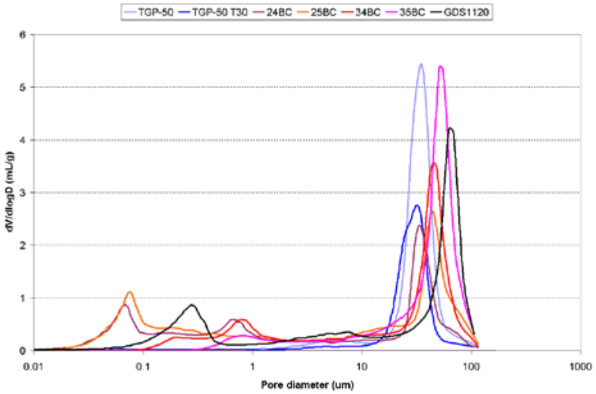
- Validated single-phase Lattice Boltzmann Model applied to screen GDL concept with oriented fibers:
  - Predicted possibility of controlling in-plane (transverse versus longitudinal) transport with fixed through-plane transport by modifying GDL microstructure
  - Experimental evaluation of similar work with experimental data supporting potential promise shown at 217th ECS meeting by Jonquille and Pauchet

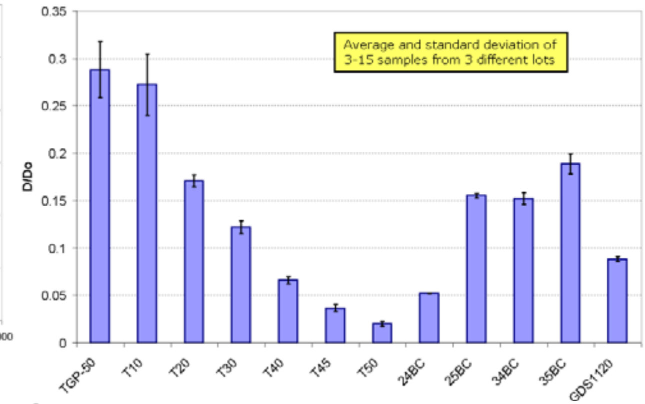


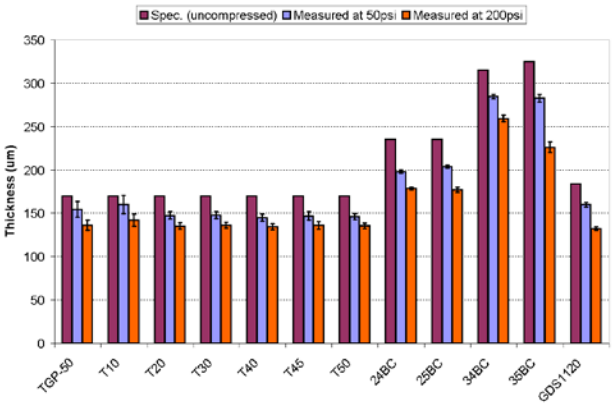


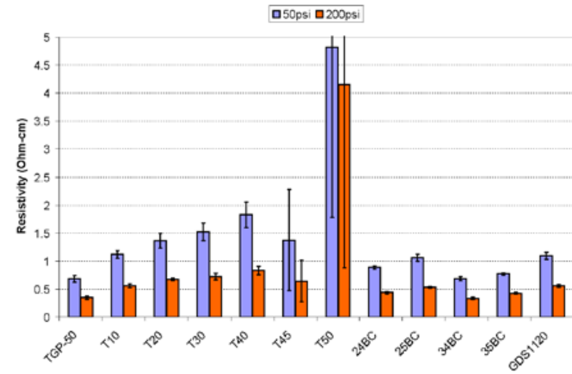
Overall Accomplishments: GDL Materials Characterization (2009)

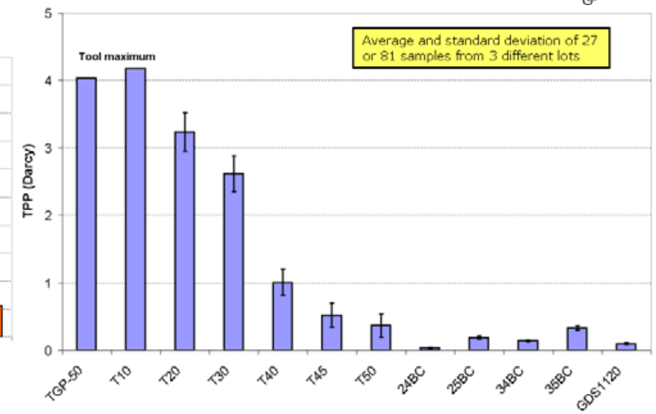






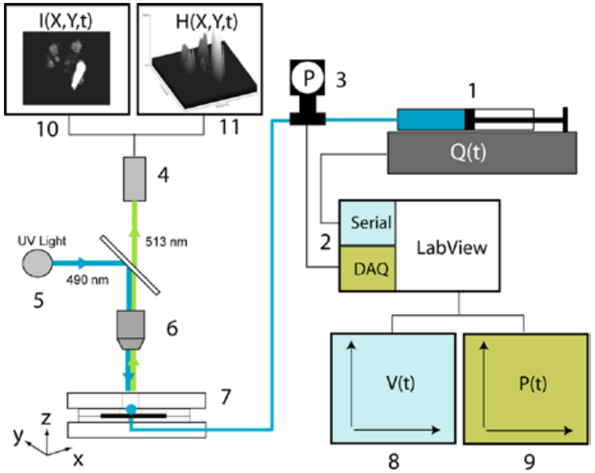






- Key property database established for SGL, BMP & Toray papers with a range of PTFE loadings (Ballard, Techverse):
  - Porosity and Pore Size Distribution (MIP, MSP)
  - In- and Through-Plane Gas Permeability, Effective Diffusivity
  - Electrical and Thermal Conductivity
  - Thickness & Electrical Resistance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

Overall Accomplishments:
GDL Water Transport Characterization and Modeling (2009)

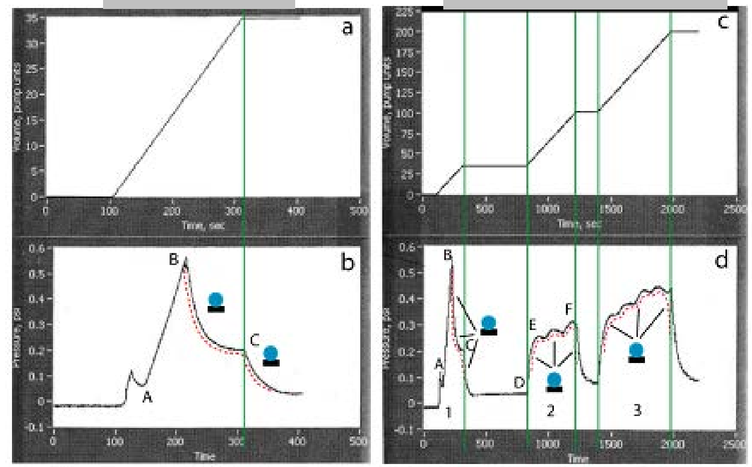


UVic *Simultaneously* monitored the development of the capillary flow, pressure, and volume injection rate of water percolating through the GDL porous layer

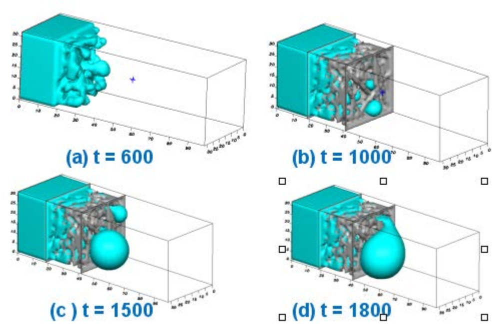
Experimental Observations

Dry Sample

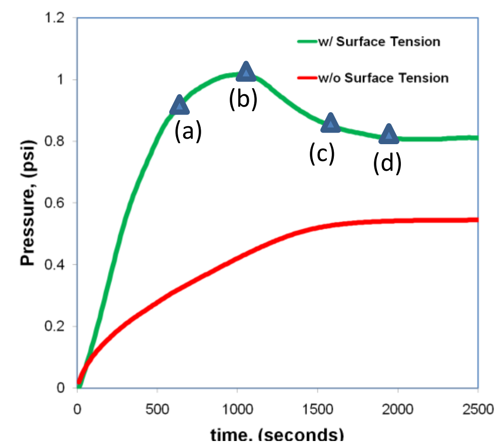
Wet Initial Sample



LBM Modeling of GDL Transport



Test GDL: porosity 0.75, thickness 100μm.



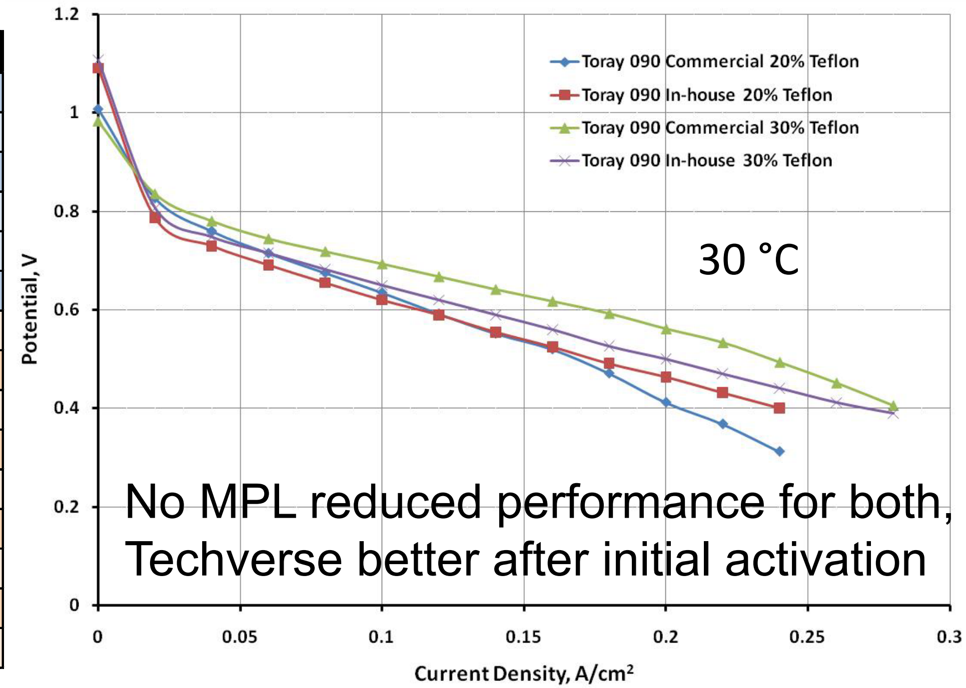
- Preferred channels for water transport, history dependent invasion observed
- 2-Phase Lattice Boltzmann Model predicted similar channeling
- Experiments and LBM guided CFD model formulation

Overall Accomplishments: Electrophoresis for Uniform GDL PTFE (2011)

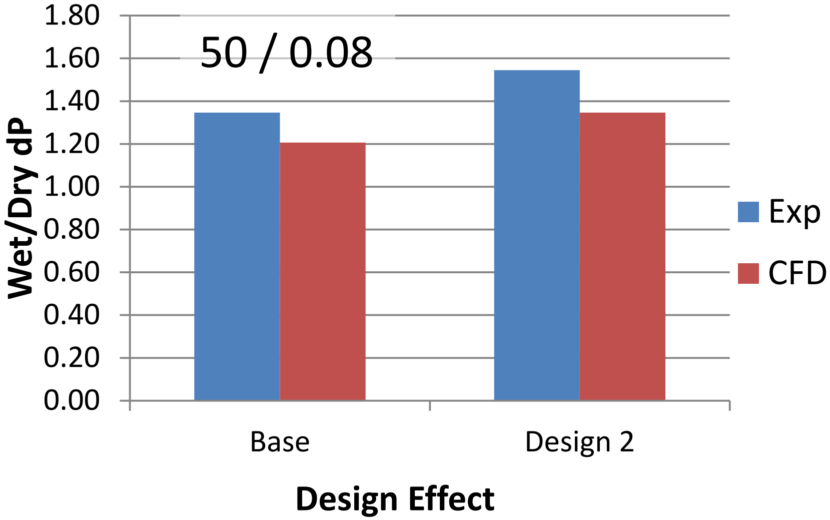
- More uniform PTFE coatings for 10x lower residual saturation (liquid water staying in the GDL), increased hydrophobicity at equivalent loadings.
- Testing at BCS Fuel Cells: Better performance than commercial media at moderate currents despite slight increase in activation losses and/or contact resistance

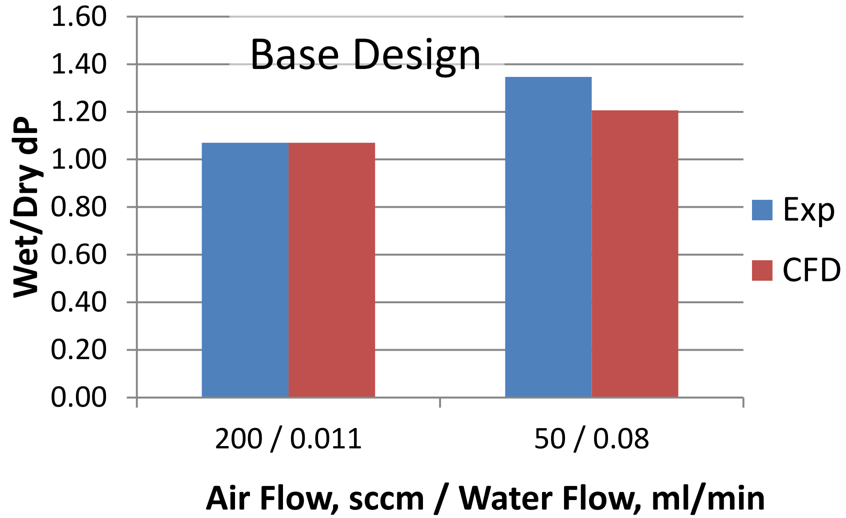
Sample	Residual Saturation	Breakthrough Pressure
n/a	%	Pa
35 EA - 30% Teflon	15.52	587
35 DA - 20% Teflon	25.54	1077
35 CA - 10% Teflon	7.6	1175
30% in-house AA sample	2.44	1959
7.5% in-house AA sample	2.32	1763
30% in-house A Toray	0.416	4800
15% in-house A Toray	0.6	3400
6% in-house A Toray	0.8	3100
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

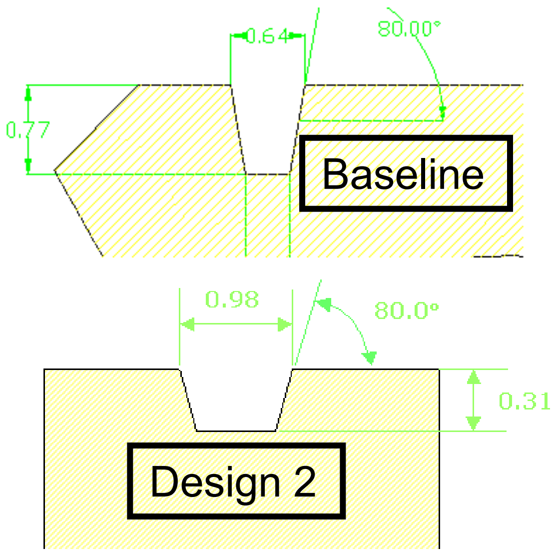
Teflon is a registered trademark of E.I. du Pont de Nemours and Company

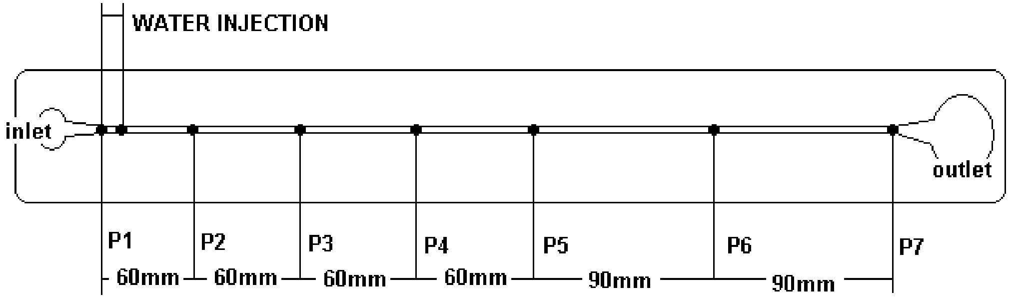


Overall Accomplishments: Two-Phase Channel dP with GDLs (2011)







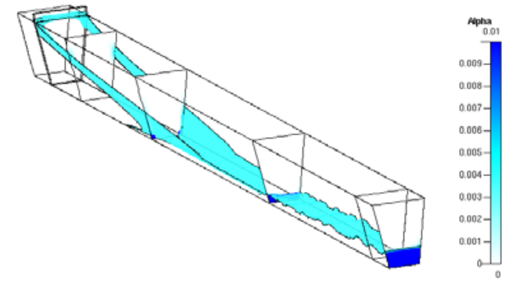


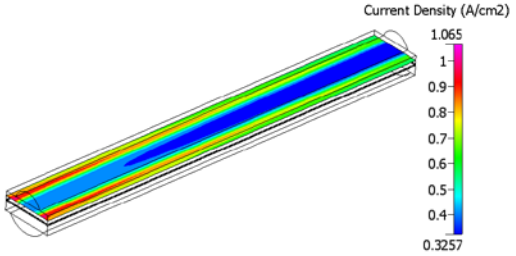
- **Ballard Two-Phase dP measurements identified designs with low wet dP and pressure fluctuations**
- **Models predicted trends with design variation and operating conditions for GDL+channel**

Overall Accomplishments: Software Package Summary

ESI is providing the developed and models into the commercial version of CFD-ACE+:

- Solver capabilities:
  - Improved two-phase flow in fuel cell scale channels, two-phase flow in porous media: demonstrated to predict predict pressure drops in fuel cell GDL+channel assemblies as function of design and operating conditions => impact of channel design and GDL properties on balance of plant requirements, system efficiency
  - Liquid water effect on effective diffusivity of reactants in GDL => impact of liquid water content and distribution on performance
  - Mass transfer between fluid phases coupled with fuel cell chemistry via electrochemical reactions and evaporation/condensation
- Model Definition
  - GUI for problem setup to specify water transport model options and input parameters (relative permeability, capillary pressure models, liquid effect on tortuosity, etc.)
- Post-Processing:
  - Printed summaries (mass, energy, and chemical species balances) and graphical output (liquid volume fraction, mass transfer rates, liquid phase velocities; in addition to overpotentials, transfer current already provided for fuel cell models)





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; continuing application of the developed models
  - 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; commercial release of the developed models
  - SGL Carbon: GDL and bipolar plate materials
  - U. Victoria: GDL permeation, channel droplet injection and transport quantification

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:
  - Developed and validated both single-phase and two-phase Lattice Boltzmann Models for flow in porous media, applied to screen microstructure design concepts and analyze fundamental characteristics of water transport in GDLs;
  - Characterized GDL materials over a broad range of PTFE treatment;
  - Developed a two-phase cell scale CFD model for analyzing cell components (channel design, GDL effective properties) and predicted cell performance; validated key sub-models for two-phase flows in channels and transport in porous media
  - 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;
  - Developed a technique for reproducible, controllable hydrophobic treatment of GDL media