CFDRC Better Decisions, Better Products Through Simulation & Innovation

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

J. Vernon Cole and Ashok Gidwani
CFDRC

Prepared for:
2007 DOE Hydrogen Program Annual Review
May 16, 2007

Project ID: FCP23

CFD Research Corporation www.cfdrc.com
215 Wynn Drive • Huntsville, Alabama 35805 • Tel: (256) 726-4800 • FAX: (256) 726-4806 • info@cfdrc.com

Overview

- **Timeline**
  - Start Date: 5/1/07 (est)
  - End Date: 4/30/11
  - Percent Complete: 0%

- **Budget**
  - Total Funding: $ 6.3 M
    - DOE Share: $5.0 M
    - Team Share: $1.3 M
  - Funding Received FY06: $0
  - Funding for FY07: $800 K

- **Barriers Addressed:**
  - A. Durability
  - 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
  - Research Triangle Institute
  - SGL Carbon
  - ESI Group, NA
  - U. Victoria

Program Objectives

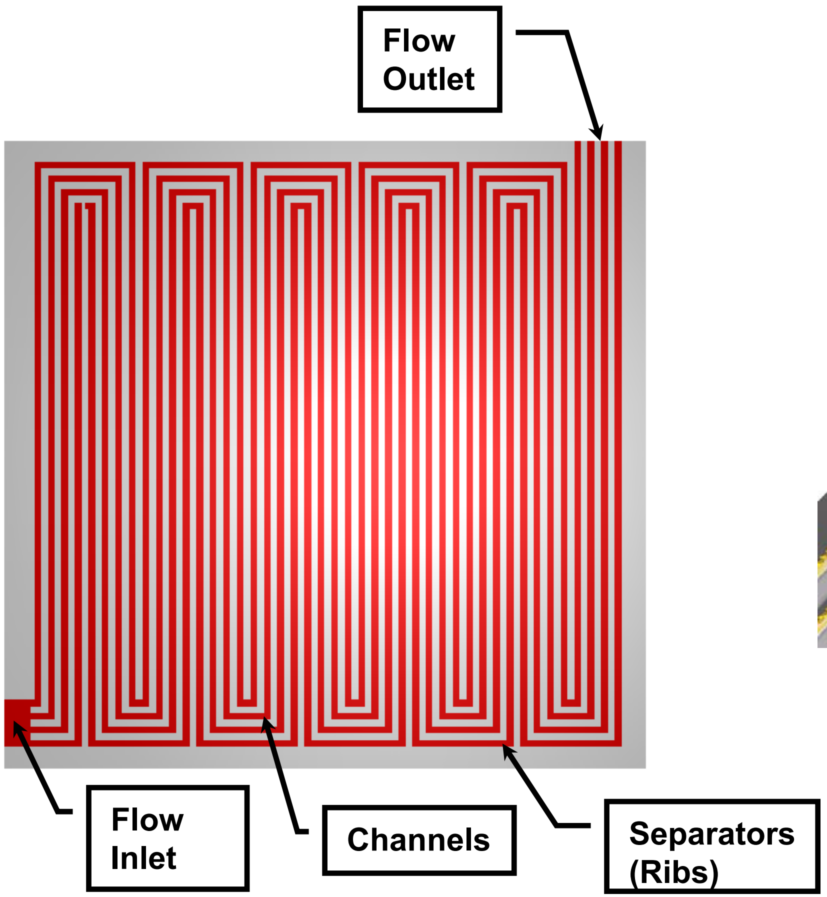
- **Overall:**
  - Develop advanced physical models and conduct material and cell characterization experiments;
  - Improve understanding of the effect of various cell component properties and structure on the gas and water transport in a PEM fuel cell;
  - Demonstrate improvements in water management in cells and short stacks; and
  - Encapsulate the developed models in a commercial modeling and analysis tool.
- **2007:**
  - 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 and begin implementing/testing improved models for transport in GDLs, channels, and across interfaces

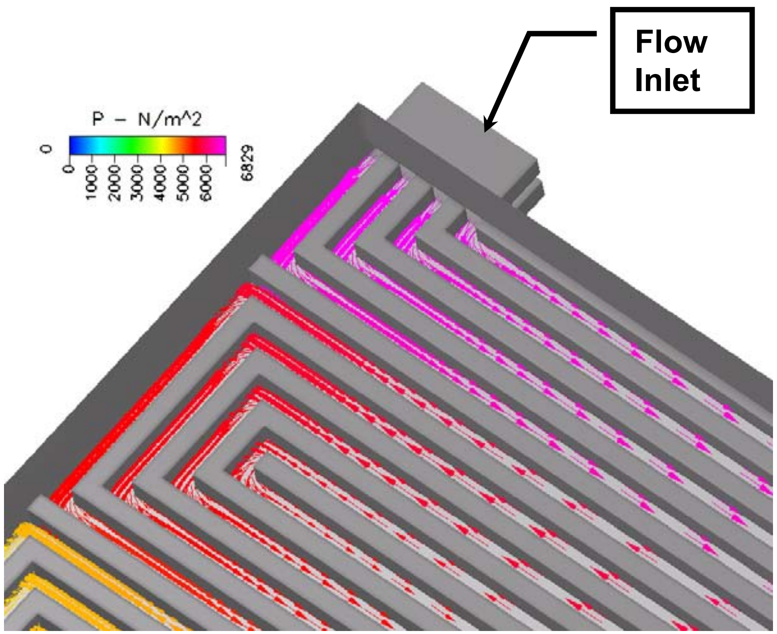
Approach

- **Overall:**
  - Integrated experimental characterization and model development
  - Systematically address each of the component regions of the cell
  - Integrate the developed advanced modeling capabilities into an analysis tool capable of addressing water transport issues in future generation cell designs
- **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

CFDRC Prior Work: Example Case

- 50 cm^2 fuel cell with 4 serpentine channels
- Three-dimensional model, ~ 1.4 million grid cells





Cell Dimensions:
Length and Width ~ 6.9 cm

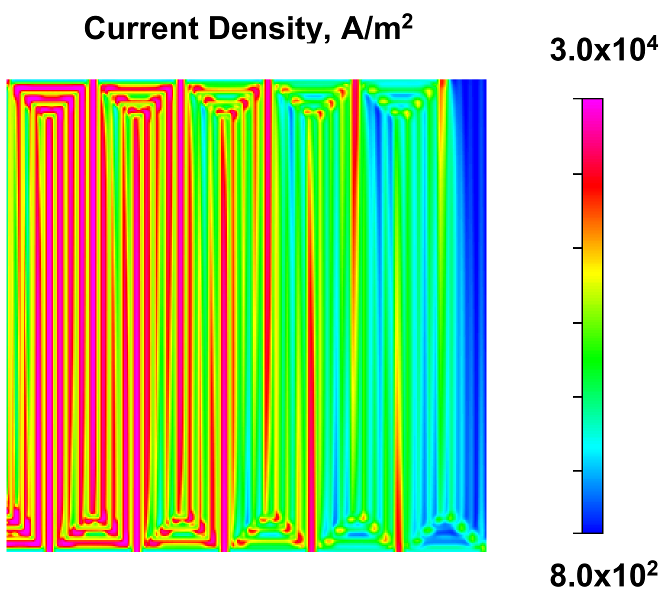
Dimensions of various layers:

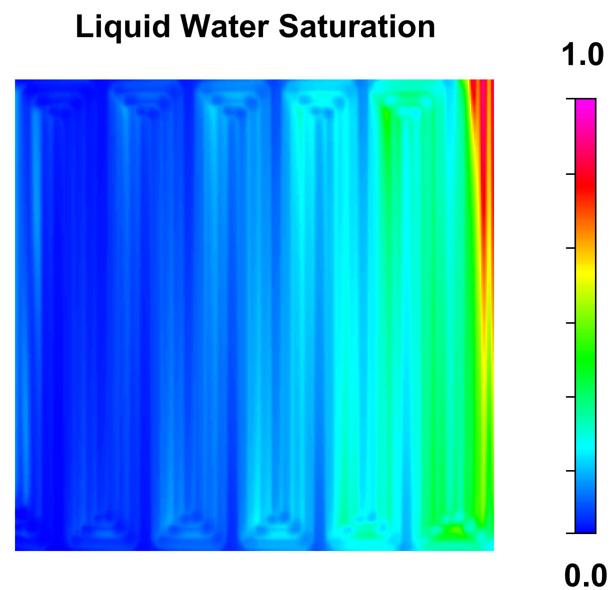
Diffusion Layer	~ 230 microns
Catalyst Layer	~ 20 microns
Membrane	~ 50 microns
Channel depth	~ 1.016 mm
Channel width	~ 0.7874 mm

DOE Hydrogen Program

CFDRC Prior Work: Sample Results

- **Operating conditions: 100% relative humidity, 80°C, 1 atm pressure, V_{cell} = 0.225 V**
- **Distributions of current density (membrane mid-section) and liquid water saturation (cathode catalyst layer midsection):**



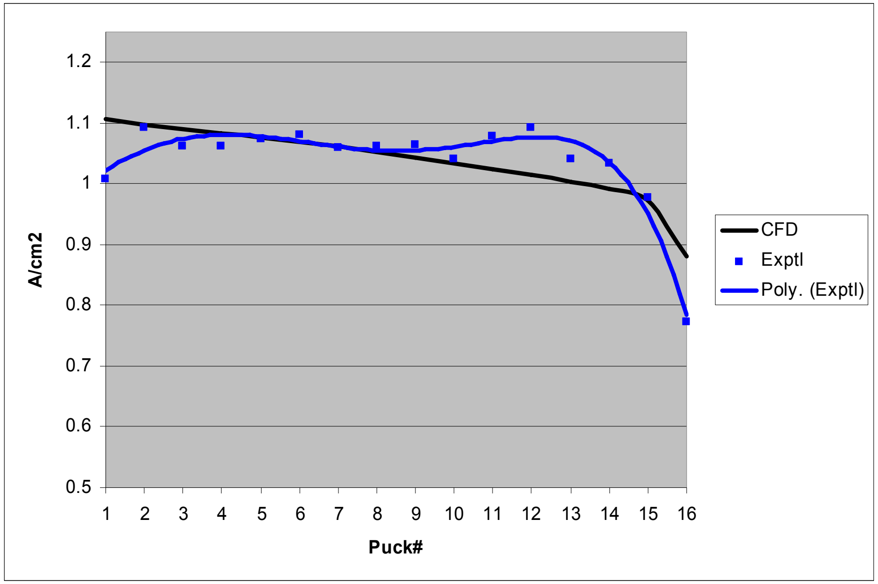


High Inlet Humidity at Low Cell Voltages Results in Larger Quantities of Liquid Saturation and Cell Flooding

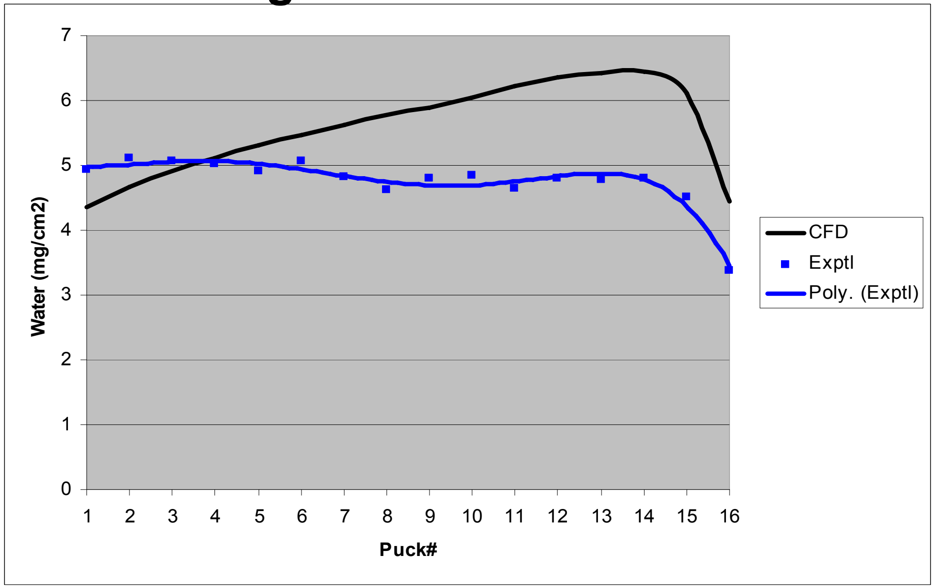
Model Testing at Ballard

Independent comparison to cell diagnostic data:

Current Distribution



MEA Water Distribution – High Current Conditions



- **High current prediction is adequate on average, but local current distribution errors are high.**
- **Predictions are poor at low current densities (needed for automotive drive cycles) and are the subject of ongoing improvement.**
- **Breakdown of MEA water into GDLs and membrane is not accurate**
- **Modeling and design of the MEA water distribution is critical to cell durability and freeze start capability**

DOE Hydrogen Program

Future Work

- **FY07:**
  - Initiate ex-situ and in-situ characterization studies
  - Finalize selection of, and begin implementing, water transport model formulation for cell and stack scale analysis
  - Initiate Lattice Boltzmann Model formulation for component-scale analysis and effective water-gas two-phase transport property prediction

- **FY08:**
  - Test improved models against ex-situ data (water and gas two-phase transport in GDL, GDL+channel)
  - Evaluate cell level model performance

- **Upcoming Milestones and Decision Points:**
  - Selection of base transport model formulation
  - Lattice Boltzmann Method evaluation and go/no-go to pursue further

Summary

- **Start has been significantly delayed:**
  - **Ongoing related research in two-phase flow and heat transfer systems will be applied to accelerate initial start-up**
  - **Schedule may need adjustment**
  - **Resource re-allocation from original plan is possible**