Better Decisions, Better Products
Through Simulation & Innovation

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

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Prepared for:
DOE Hydrogen Fuel Cell Kickoff Meeting

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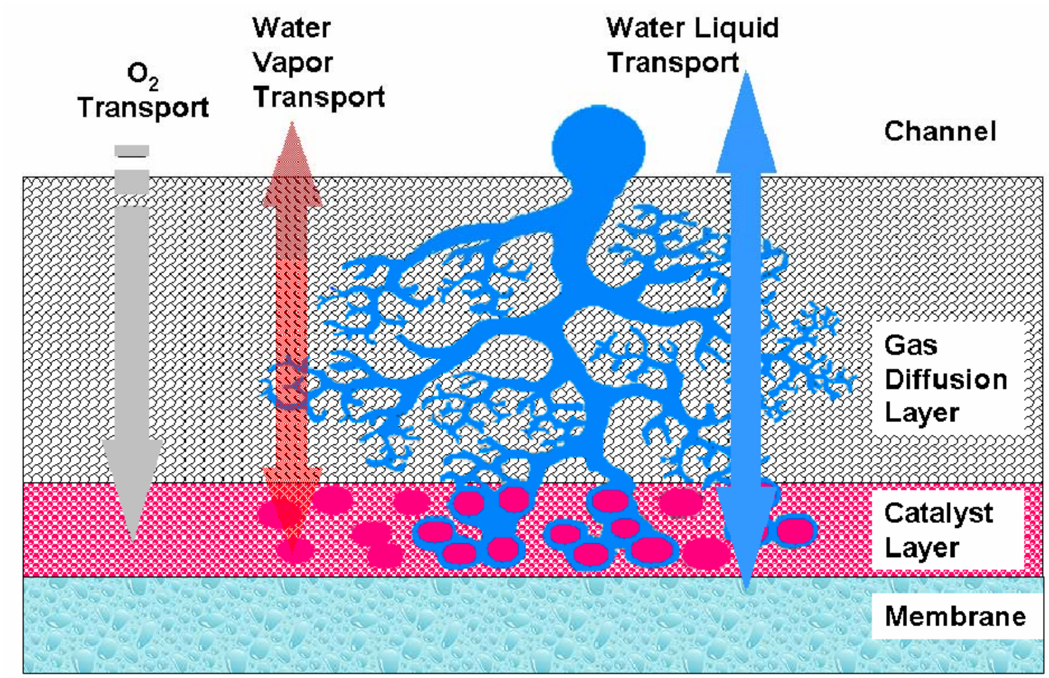
Background

Water Management Issues Arise From:

- **Generation of water by cathodic reaction**
- **Membrane humidification requirements**
- **Capillary pressure driven transport through porous MEA and GDL materials**
- **Scaling bipolar plate channel dimensions**



J.H. Nam and M. Kaviany, Int. J. Heat Mass Transfer, 46, pp. 4595-4611 (2003)

Relevant Barriers and Targets

- **Improved Gas Diffusion Layer, Flow Fields, Membrane Electrode Assemblies Needed to Improve Water Management:**
  - **Flooding blocks reactant transport**
  - **Drying out of membrane reduces protonic conductivity**
  - **Water distribution at shutdown, and transport during start-up, affects transient response, cold-start capability, and materials requirements for freeze-thaw cycle robustness**

- **Water management improvements are needed to maintain advances in transient response and cold start-up time, while improving power performance (650 W/L power density by 2010)**

Program Objectives

- **Develop advanced physical models and conduct material and cell characterization experiments to improve and optimize fuel cell design and operation;**
- **Demonstrate improvements in water management resulting in improved efficiency during automotive drive cycles, freeze/thaw cycle tolerance, and faster cold startup;**
- **Improve understanding of the effect of various cell component properties and structure on the gas and water transport in a PEM fuel cell, particularly the gas diffusion media (GDM) and flow channels; and**
- **Encapsulate the developed models in a commercial modeling and analysis tool, allowing transfer of technology to the industry for future applications.**

Approach

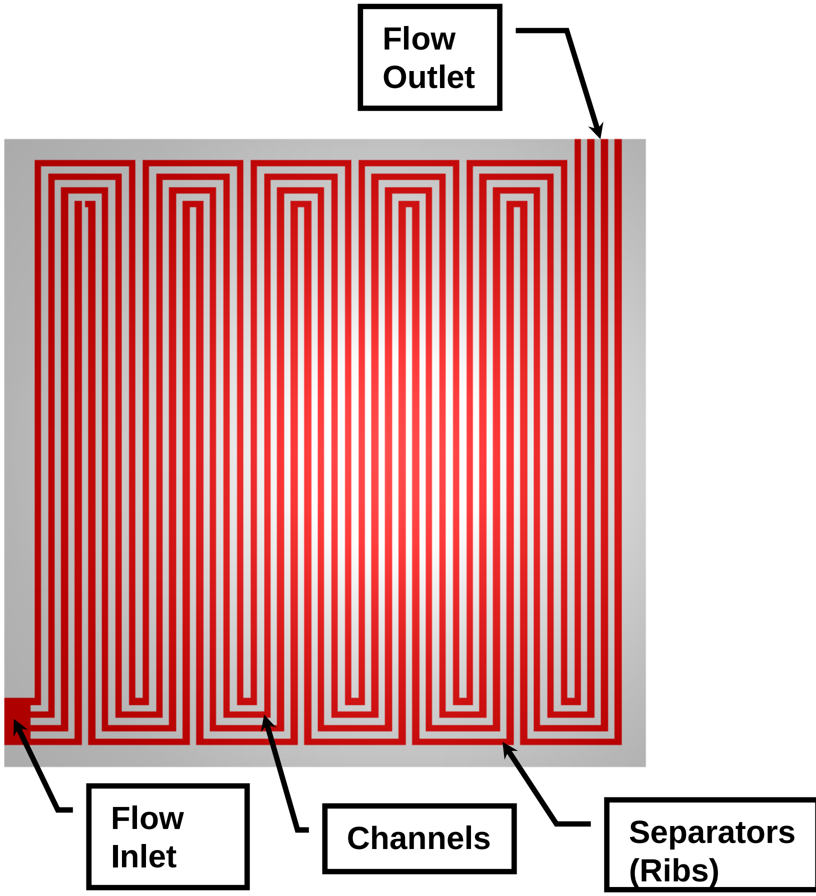
- **Overall:**
  - Integrated experimental characterization and model development
  - Systematically address each of the component regions of the cell
  - Integrate the developed advanced modeling capabilities into an analysis tool capable of addressing water transport issues in future generation cell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

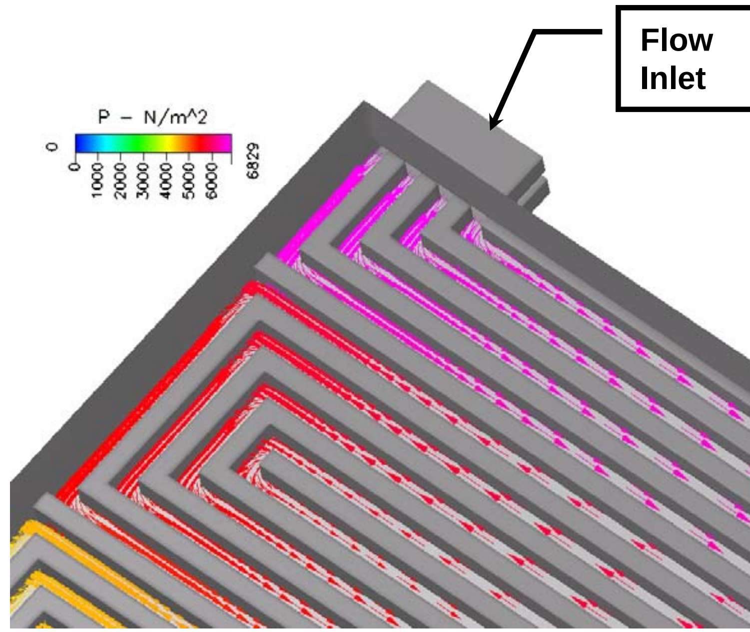
- **Modeling Approach:**
  - Develop advanced models for water transport, and model parameters, in cell component materials
  - Evaluate, and verify the developed models and parameters in a CFD based simulation tool for unit cell performance simulation
  - Apply verified modeling capabilities and simulation 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**





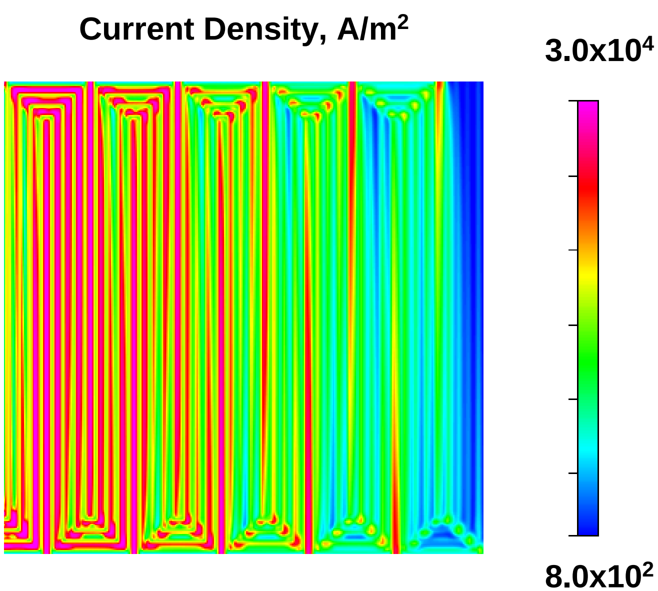
Cell Dimensions:
Length and Width ~ 6.9 cm

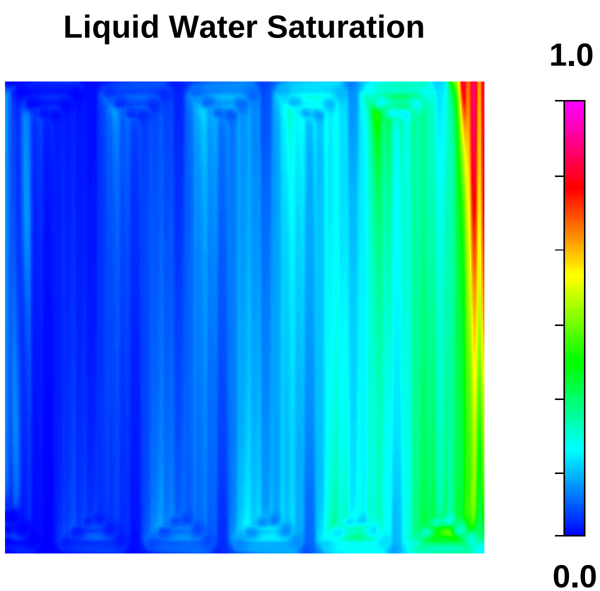
Dimensions of various layers:

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

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):



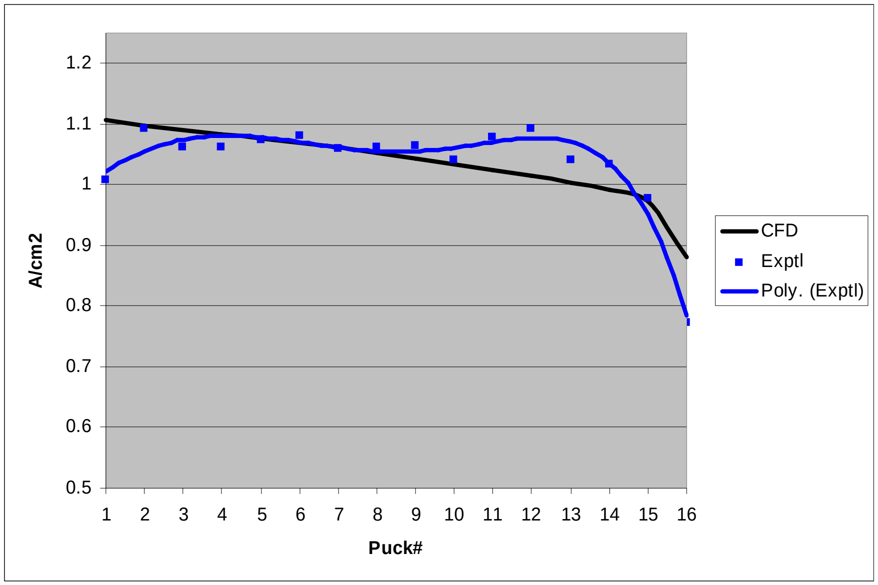


High Inlet Humidity at Low Cell Voltages Results in Larger Quantities of Liquid Saturation and Cell Flooding

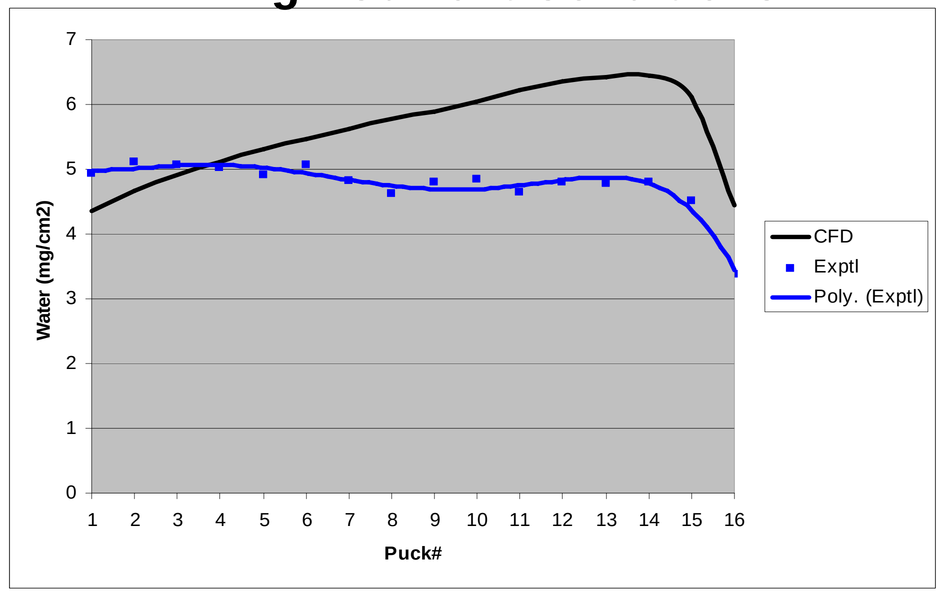
Model Testing at Ballard

Independent comparison to cell diagnostic data:

Current Distribution

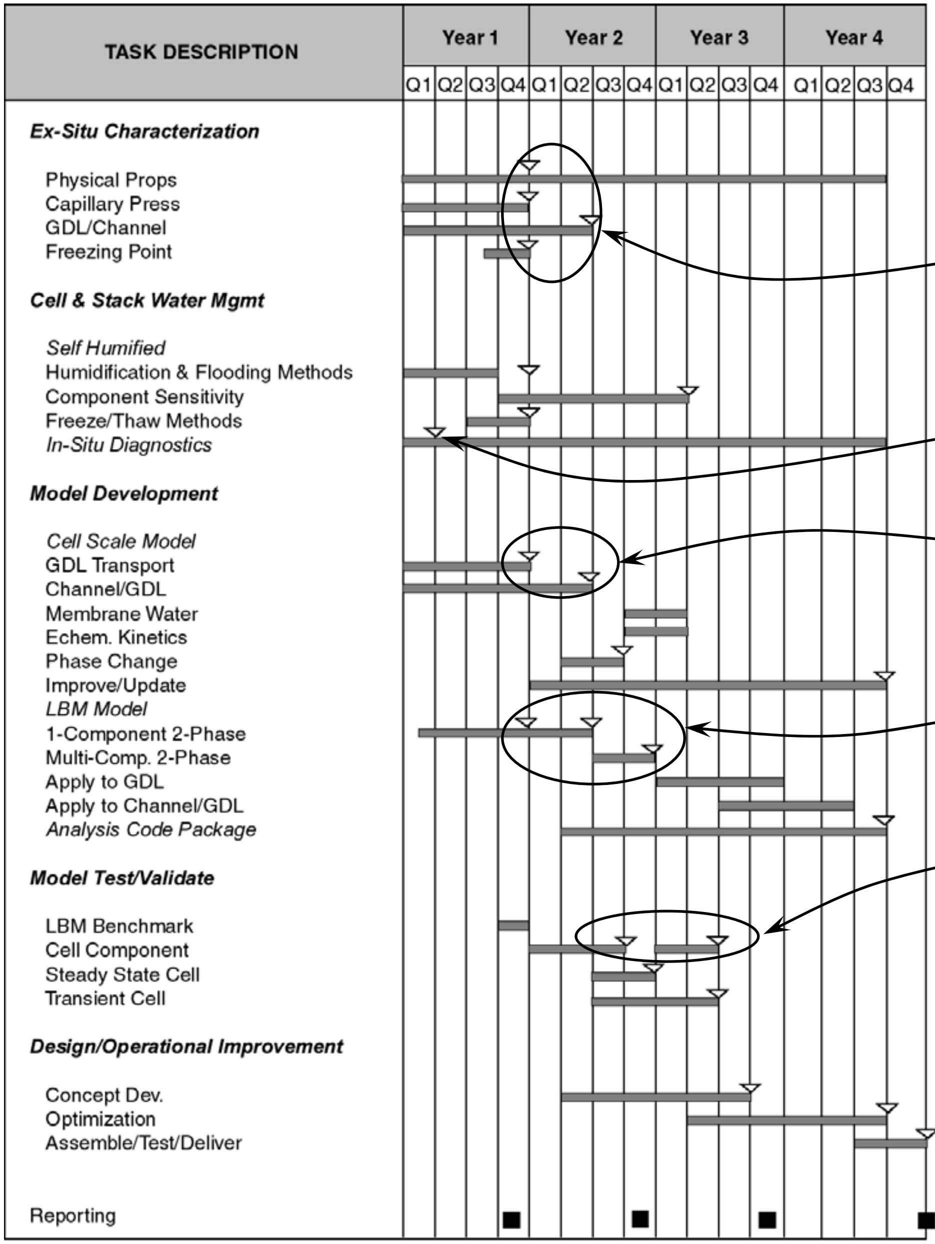


MEA Water Distribution – High Current Conditions



- **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**

Work Schedule and Milestones



Estimated Start Date: April 1, 2007

- **Ex-Situ Characterization:**
  - **Baseline material properties**
- **Cell and Stack Characterization**
  - **Initial data delivery**
- **Model Development:**
  - **Physical models down-selected and implemented**
  - **LBM coded and ready for test**
- **Model Test/Validate**
  - **Single and Multi-Component LBM**
  - **Establish confidence levels for application / need for model and parameter improvements / optional models**
- **Optimization and Demonstration**
  - **Deliver demonstration Stack**

Key Decision Points

- **Cell Scale Model Development:**
  - FY07 Q3 (Jun 2007): Down-select basic transport model formulation
  - FY09 Q1 (Dec 2008): Go/NoGo Decision for improving/extending membrane water transport and electrochemical kinetics based on outcome of steady-state and initial transient testing
- **LBM Model Development:**
  - FY08 Q2 (Mar 2008): Go/NoGo for continued development and extension to multi-component
  - FY08 Q4 (Sep 2008): Go/NoGo for continued activity (begin application)
- **Design/Operational/Materials Improvement:**
  - FY09 Q2 (Mar 2009): Select (3) candidate strategies for additional screening via simulation and additional experiments

Organization

DOE Program Monitors
- Nancy L. Garland
- Reginald Tyler

Project Management
- Vernon Cole – Program Manager
- Ashok Gidwani – Principal Investigator

Advisory Committee
- Ashok Singhal – CFDRC
- John Kenna – Ballard
- Greg Jackson – U. Maryland

Material Charact., Ex-Situ Expts.
- SGL Carbon
- Research Triangle Institute
- Ballard Power Systems
- Univ TBD

Numerical Model Dev.
- CFDRC
- ESI Group
- Ballard

In-Situ Cell Expts.
- BCS Fuel Cells
- Ballard

Model Validation
- CFDRC
- ESI
- Ballard

Design Improvements
- CFDRC
- BCS
- RTI
- SGL

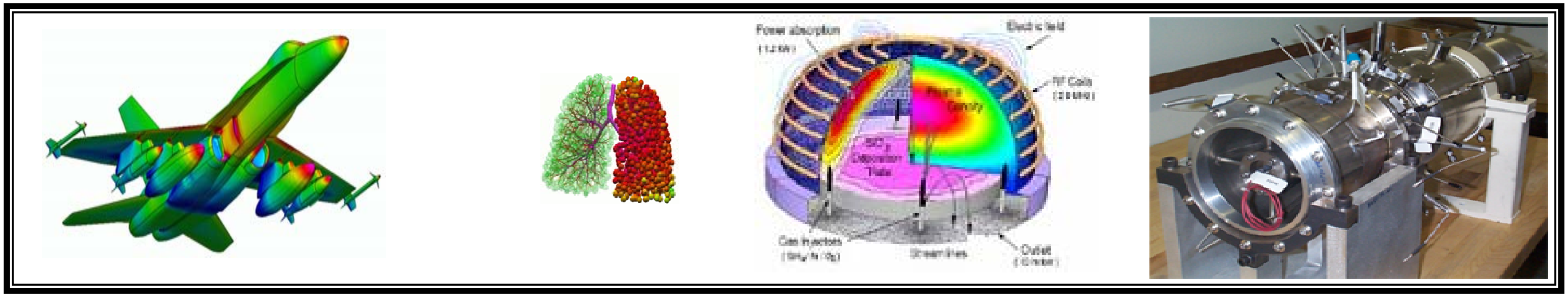
Budget Summary

By Fiscal Year:

	FY07	FY08	FY09	FY10	FY11
DOE Cost, $K	591	1,184	1,181	1,153	565
Cost Shared, $K	170	340	340	340	170
Total Budget, $K	761	1,524	1,521	1,493	735

- **Total Budget $6.03M,**
- **DOE Funding $4.7M,**
- **22% of costs shared by team**

Corporate Overview



Multi-Disciplinary Engineering Solutions

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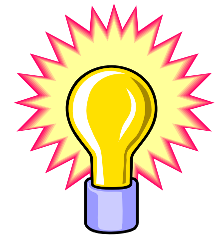
Our Approach

Physics-Based Simulations

→ **Better Insights**

→ **Better Decisions** for:



- New Designs
- Concepts
- Operations
- Safety

Simulations & Experiments

→ **Innovative Designs & Prototypes**

→ **Better Products** with:

- Greater Functionality
- Reduced Costs
- Shorter Time to Market
- Lower Risk

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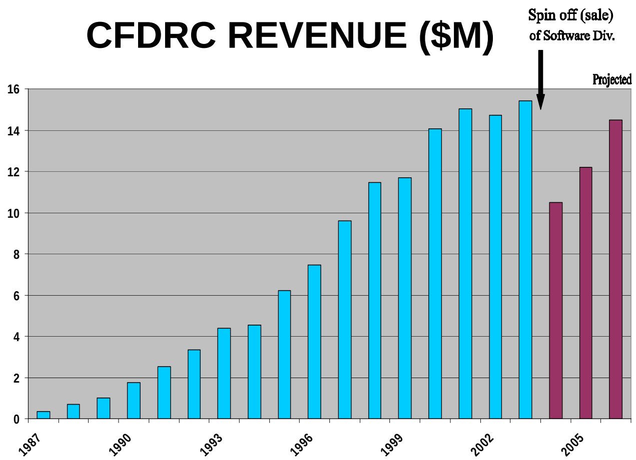
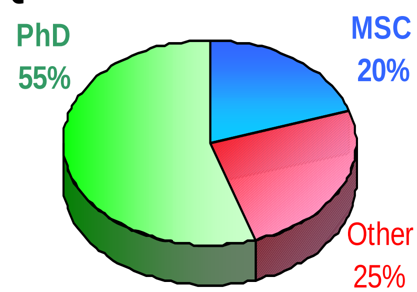
Track Record

CFDRC REVENUE ($M)

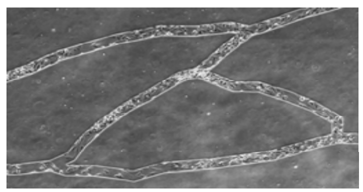


QUALIFIED PERSONNEL

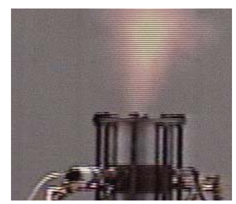


Over 25 Patents (For Licensing and Customization)

Metered Dose Inhaler Spacer

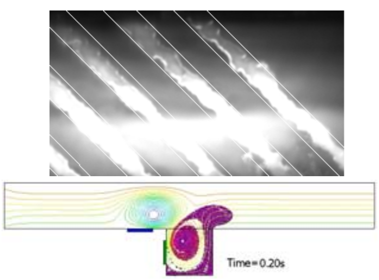


Synthetic Microvascular Networks

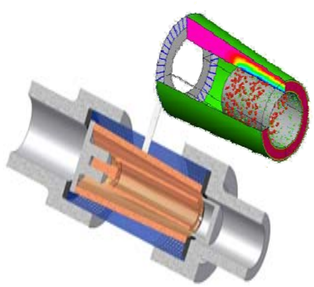


Constant Volume Rocket Motor

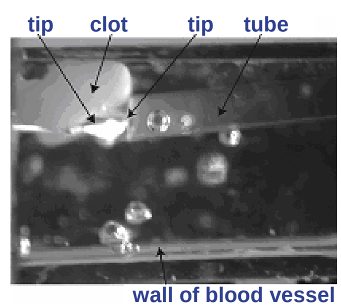
High Energy Hypergolic Bipropellant Gels



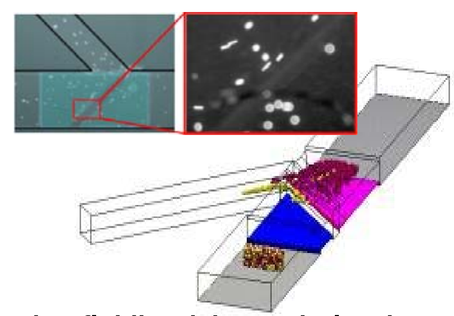
Dielectrophoresis Cell Sorter



Electrostatic Air Sampler



Thrombectomy Catheter



Microfluidic Mixing and Cleaning