



For presentation at the Fuel Cell Projects Kickoff Meeting, DOE SAND2009-5953C  
Washington DC, September 30 – October 1, 2009.

# Development and Validation of a Two-phase, Three-dimensional Model for PEM Fuel Cells

**Fuel Cell Projects Kickoff Meeting**

September 30 – October 1, 2009

Presented by: **Ken S. Chen (PI)**

**Solicitation Partners:**

**Sandia National Laboratories (Prime Applicant)**

**Pennsylvania State University**

**Lawrence Berkeley National Laboratory**

**Los Alamos National Laboratory**

**Ballard Power Systems**

**Ford Motor Company**

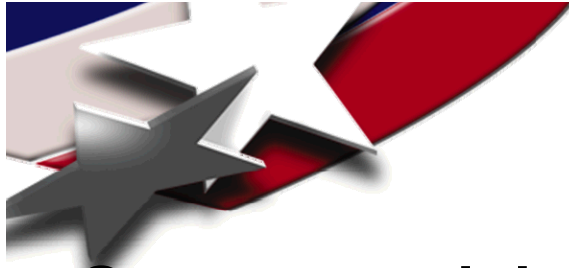


# Objectives

- To develop and validate a **two-phase, three-dimensional transport model** for simulating PEM fuel cell performance under a **wide range of operating conditions**.
- To apply the validated PEM fuel cell model to **improve fundamental understanding** of key phenomena involved and to **identify rate-limiting steps** and **develop recommendations for improvements** so as to accelerate the commercialization of fuel cell technology.
- The validated transport model can be employed to improve and optimize PEM fuel cell operation. Consequently, the project helps:  
i) **address the technical barriers on performance, cost, and durability;**  
and ii) **achieve DOE's near-term technical targets on performance, cost, and durability in automotive and stationary applications.**

## DOE 2015 (Automotive) and 2011 (Stationary) Technical Targets

	Performance	Cost	Durability
Automotive (2015)	650 W/L or 50% energy efficiency	\$30/kW	5,000 hours
Stationary (2011)	40% electrical energy efficiency	\$750/kW	40,000 hours



# Approach

Our approach is both **computational** and **experimental**:

- Numerically, develop a **two-phase, 3-D, transport model** for simulating PEM fuel cell performance under a wide range of operating conditions.
- Experimentally, measure **model-input parameters** and generate **model-validation data**.
- **Perform model validation** using experimental data available from the literature and those generated from team members.
- Apply the validated transport model to **identify rate-limiting steps** and **develop recommendations** for improvements.

A staged approach will be adopted in model development and validation:

**Single phase (dry) → Partially two-phase (dry-to-wet transition) → Fully two phase (wet)**



# Relevant Prior Work

**Many PEM fuel cell models (mostly piece-wise) have been published:**

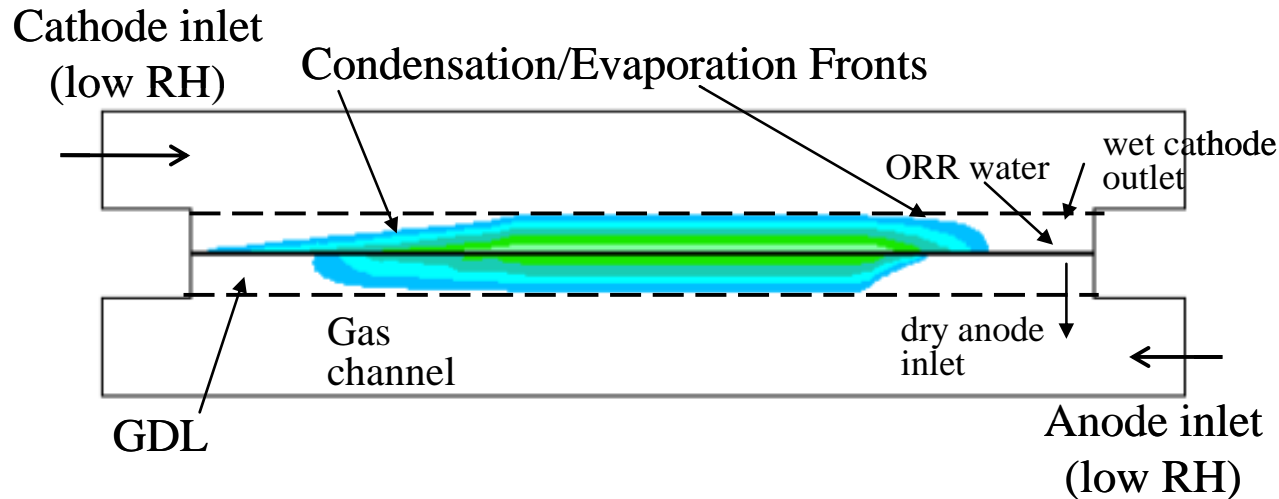
- **Simple 1-D models:** e.g., Springer et al. (1991), Bernardi and Verbrugge (1992)
- **2-D models:** e.g., Nguyen and White (1993), Gurau et al. (1998), Um et al. (2000)
- **Quasi 3-D models:** e.g., Kulikovskiy (2003), Muller et al. (2007)
- **3-D models:** e.g., Dutta et al. (2000), Zhou and Liu (2001), Berning et al. (2002), Mazumder & Cole (2003a), Li & Becker (2004), Um & Wang (2004), Lum and McGuirk (2005), Hu and Fan (2006), Meng (2006)
- **Reduced dimen. stack models:** e.g., Chang et al. (2007), Freunberger et al. (2008)

**The published models can also be classified as single-phase or two-phase:**

- **Single-phase:** e.g., Dutta et al. (2000), Um et al. (2000), Mazumder & Cole (2003a)
- **Two-phase:** e.g., Wang et al. (2001), Natarajan & Nguyen (2001), You & Liu (2002), Berning and Djilali (2003), Mazumder and Cole (2003b), Weber et al. (2004), Pasaogullari and Wang (2004), Meng and Wang (2005)

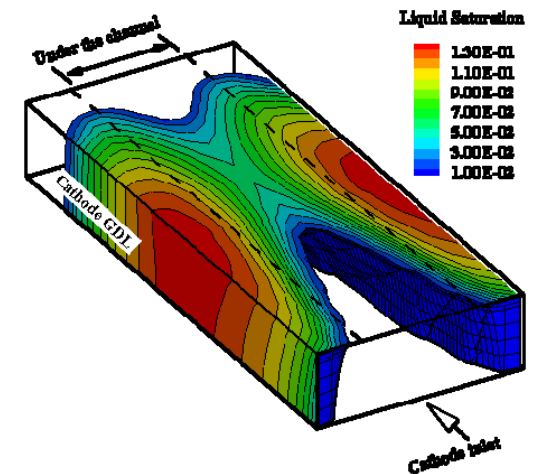
**Two big deficiencies of prior models:** 1) **piece-wise** (treat only some components)  
2) **narrow range of operating conditions**  
(e.g., either very dry or fully humidified)

**Approach: Develop a unified model and computer code for a wide range of operating conditions (dry, dry-wet, and wet)**

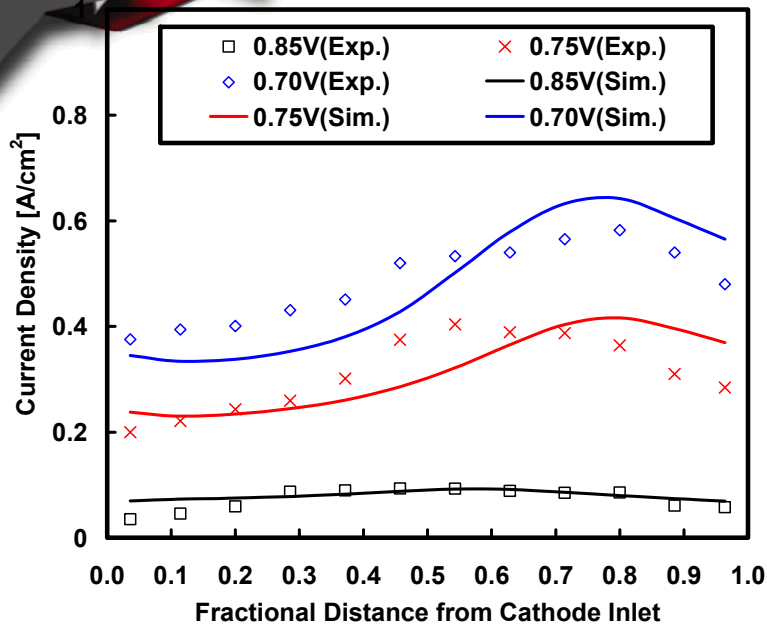


Luo, Ju, and Wang,  
*J. Electrochem Soc.*,  
**154**, B316-B321(2007)

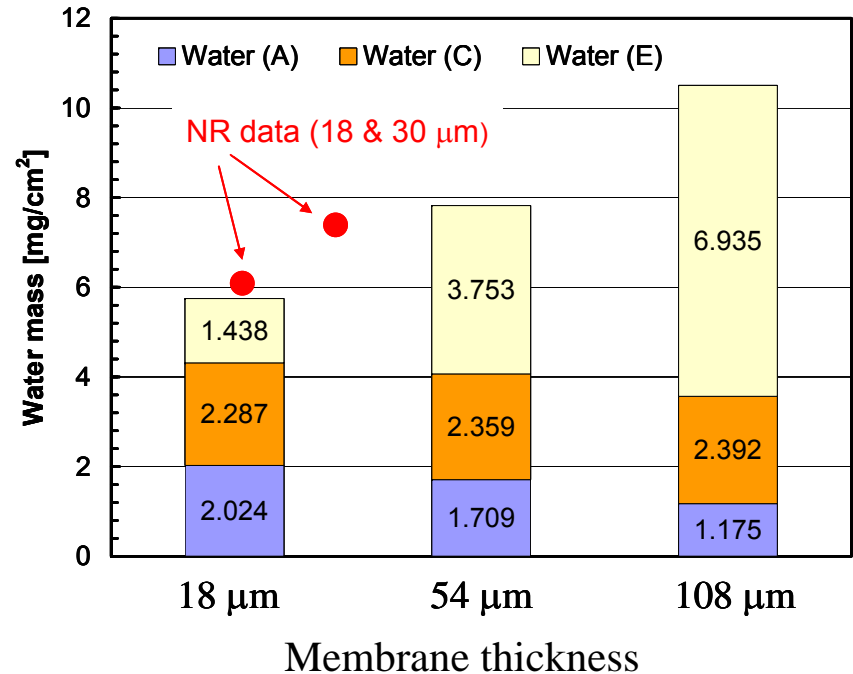
- **Dry-to-wet transition (moving boundary) inside fuel cells is the greatest challenge of water management modeling.**
- Prior work (Luo et al., JES 2007) developed a basic numerical model for single straight-channel fuel cells.
- **Developing a comprehensive numerical model for commercial-scale, complex flowfield fuel cells will be attempted in this project.**



## Approach: Compare model predictions with spatially-resolved experimental measurements



Ju et al., JES, **152**, A1645-A1633 (2005)



- **Single-phase model predictions have been validated by current-distribution data with good agreement.**
- **Under two-phase conditions, total water content in PEM fuel cells has also been validated against neutron radiography (NR) data.**
- **This project will attempt comparison of cross-sectional water distributions measured by neutron imaging and predicted by two-phase PEM fuel cell model.**



## Approach: areas for model improvements

- Water and proton transport in membrane under a wide range of water content
- Water transport mechanism(s) and structure-transport relationship in catalyst layers
- Liquid-water transport with condensation or evaporation in gas diffusion layers (GDLs) and microporous layers (MPLs)
- Water-flux interfacial condition at the GDL/channel interfaces
- Two-phase (liquid and gas) flow in gas flow channels
- Integration of sub-models into a coherent cell model
- Numerical efficiency and model robustness
- Stack models with higher fidelity (e.g., full dimensions)
- More rigorous and complete model validation
- Uncertainty analyses





# List of milestones

Task/org	Year/Qtr	Symbol	Description
1/SNL, PSU, LBNL	PY1/Q4	M1	Develop a 3-D, partially two-phase, single-cell model
2/LANL, PSU, Ballard, Ford	PY1/Q4	M2	Measure model-input parameters and generate model-validation data for single-phase operating regime
1/SNL, PSU, LBNL	PY2/Q4	M3	Develop a 3-D, fully two-phase, single-cell model
2/LANL, PSU, Ballard, Ford	PY2/Q3	M4	Measure model-input parameters and generate model-validation data for partially two-phase operating regime
3/PSU, SNL, Ballard, Ford	PY2/Q4	M5	Perform validation of the 3-D, partially two-phase, single-cell model
1/LBNL, PSU, SNL	PY3/Q4	M6	Complete development of physical/electrochemical, mathematical, sub-models
1/PSU, SNL, LBNL	PY3/Q4	M7	Complete numerical implementation and algorithm development
1/PSU, SNL	PY3/Q4	M8	Develop a 3-D, two-phase, short-stack model
2/LANL, PSU, Ballard, Ford	PY3/Q4	M9	Measure model-input parameters and generate model-validation data for fully two-phase operating regime
3/PSU, SNL, Ballard, Ford	PY3/Q4	M10	Perform validation of 3-D, fully two-phase, single-cell model
3/PSU, SNL, Ballard, Ford	PY4/Q2	M11	Perform validation of 3-D, two-phase, short-stack model
4/Ballard, Ford, PSU, SNL, LBNL	PY4/Q3	M12	Identify rate-limiting steps and develop recommendations for improvements in stationary and transportation and applications
5/SNL, PSU, LBNL, LANL, Ballard, Ford	PY4/Q4	M13	Disseminate and document models, and compile data generated during model development and validation



# Go/no-go decision points

## FY10/Q4:

**Go/no-go (G1): determine whether or not we should proceed to develop a 3-D, fully two-phase, single-cell model.**

- A **go** decision means that we shall proceed to develop a 3-D, fully two-phase, single-cell model.
- A **no-go** decision means either we go back to improve the sub-models or discontinue the project.

## FY11/Q4:

**Go/no-go (G2): determine whether or not we should proceed to develop a 3-D, two-phase, short-stack model.**

- A **go** decision means that we shall proceed to develop a 3-D, two-phase, short-stack model.
- A **no-go** decision means either we go back to improve the sub-models or discontinue the project.

## FY12/Q4:

**Go/no-go (G3): determine whether or not we should proceed to identify rate-limiting steps and develop recommendations for improvements in both automotive and stationary applications.**

- A **go** decision means that we shall proceed to identify rate-limiting steps and develop recommendations for improvements in both automotive and stationary applications.
- A **no-go** decision means either we go back to improve the models or discontinue the project.



# Organizations Responsible for Project Work

## **Sandia National Laboratories**

(Project Lead; model development, integration, testing, validation, dissemination)

## **Pennsylvania State University**

(Model development, validation, and dissemination; numerical implementation; flow property measurements; optimization studies)

## **Lawrence Berkeley National Laboratory**

(Sub-model development, including membrane and GDL/GFC boundaries; model dissemination)

## **Los Alamos National Laboratory**

(Input parameter measurements, model-validation data generation)

## **Ballard Power Systems**

(Input parameter, model-validation data and runs for stationary applications)

## **Ford Motor Company**

(Guidance and recommendations of improvements for automotive applications)

# Budget

## FY09–FY10

**Total (federal & matching): \$1484K**

subtotal (federal): \$1390K

subtotal (matching): \$94K

**SNL (federal): \$685K**

**PSU and Ballard (federal): \$375K**

**PSU & Ballard (matching): \$94K**

**LANL and LBNL (federal): \$330K**

## FY12

**Total (federal & matching): \$1408K**

subtotal (federal): \$1305K

subtotal (matching): \$103K

**SNL (federal): \$563K**

**PSU and Ballard (federal): \$412K**

**PSU & Ballard (matching): \$103K**

**LANL and LBNL (federal): \$330K**

## FY11

**Total (federal & matching): \$1419K**

subtotal (federal): \$1316K

subtotal (matching): \$103K

**SNL (federal): \$574K**

**PSU and Ballard (federal): \$412K**

**PSU & Ballard (matching): \$103K**

**LANL and LBNL (federal): \$330K**

## FY13

**Total (federal & matching): \$1180K**

subtotal (federal): \$1081K

subtotal (matching): \$99K

**SNL (federal): \$475K**

**PSU and Ballard (federal): \$396K**

**PSU & Ballard (matching): \$99K**

**LANL and LBNL (federal): \$210K**

**Total project funding over 4 years: \$5491K (federal: \$5092K; cost share: \$399K)**



# Backup Vugraphs



# Project Personnel or Participants

## **Sandia National Laboratories:**

**Ken Chen, Brain Carnes**

## **Pennsylvania State University:**

**Chao-Yang Wang, Christian Schaffer, Fangming Jiang, Gang Luo, Yan Ji**

## **Lawrence Berkeley National Laboratory:**

**Adam Weber**

## **Los Alamos National Laboratory:**

**Rod Borup, Rangachary Mukundan**

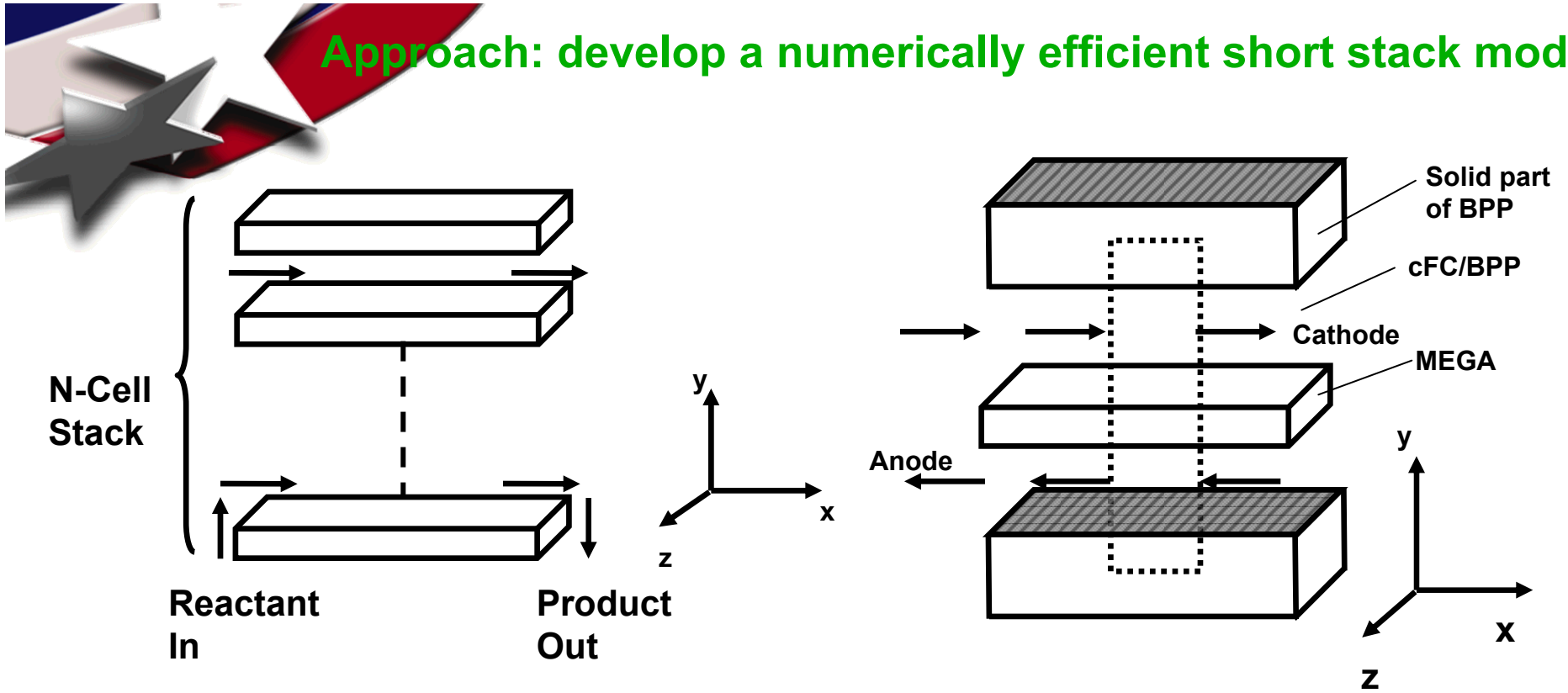
## **Ballard Power Systems:**

**Silvia Wessel, David Harvey**

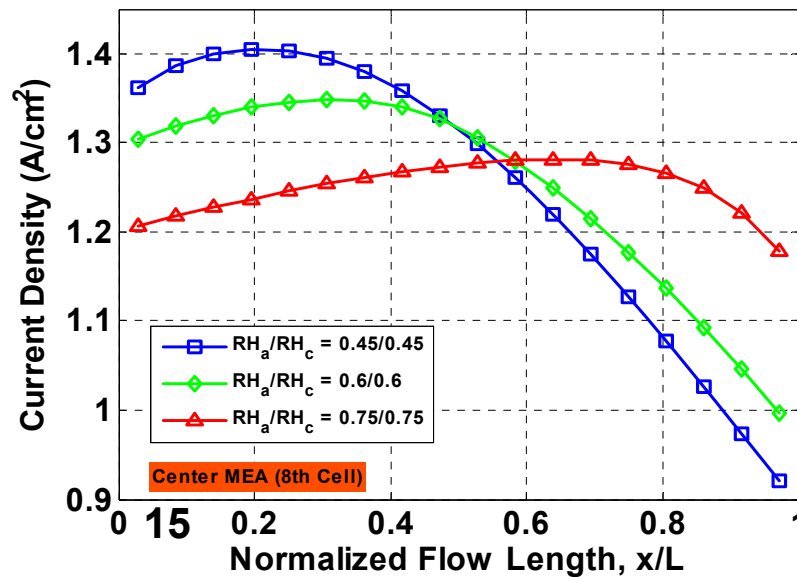
## **Ford Motor Company:**

**Ron Brost**

# Approach: develop a numerically efficient short stack model

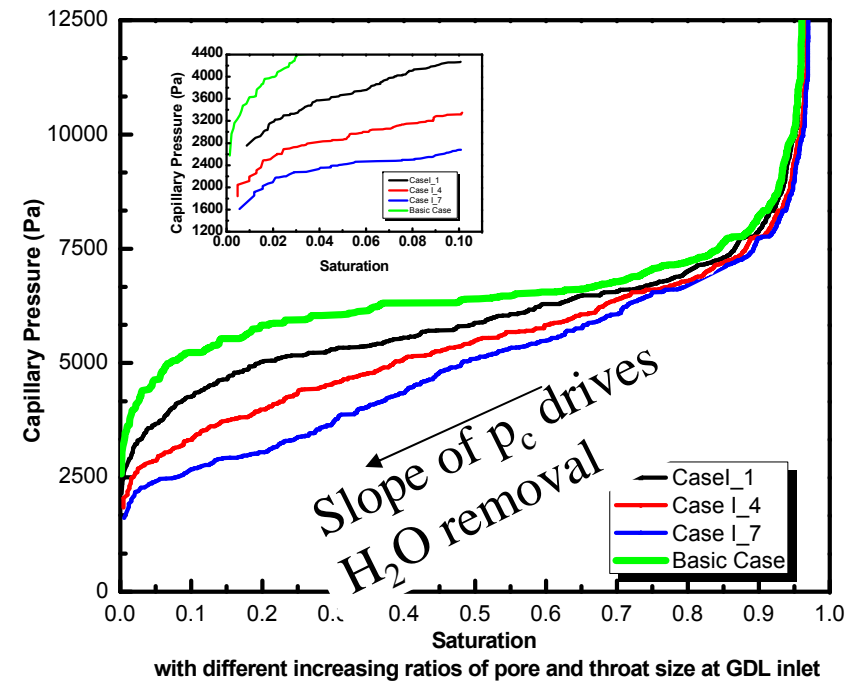
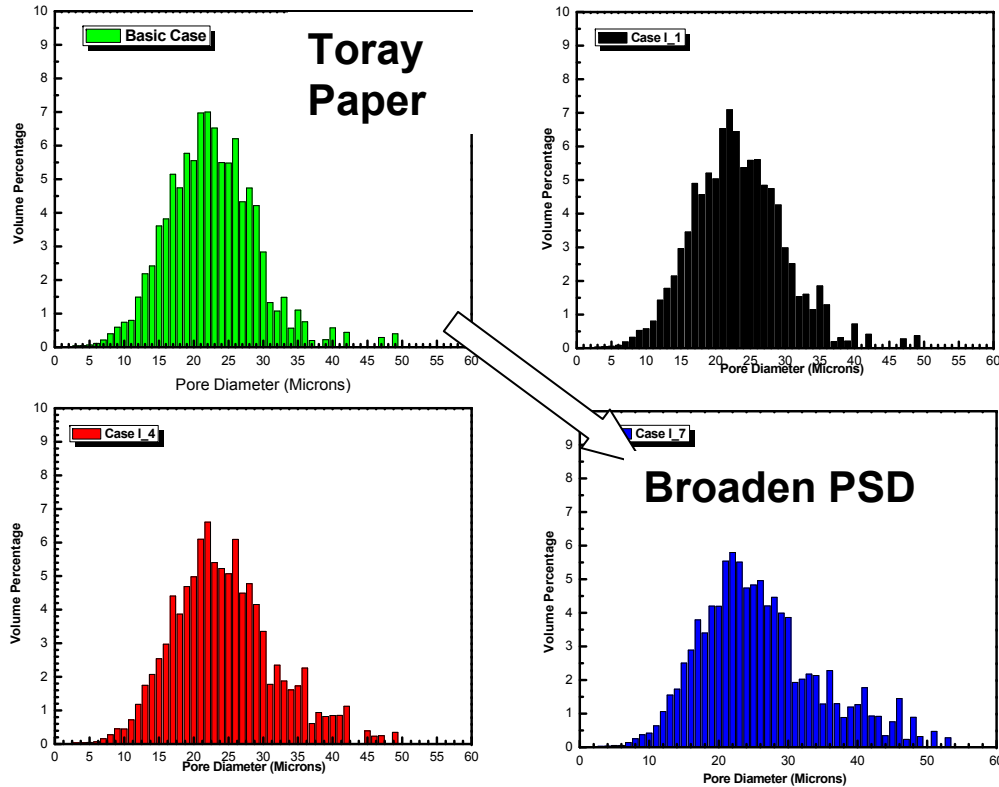


- Goal: predict flow maldistribution, cell imbalance, end cell effects etc. in a multi-cell stack





## Approach: Address relationships among GDL pore structure, transport properties and cell performance (I)



Two-phase transport properties of GDL,  $p_c$  and  $k_r$ , predicted by topologically equivalent pore network (TEPN) model (Sinha & Wang, ECS Fall Mtg, 2008)

# Approach: Address relationships among GDL pore structure, transport properties and cell performance (II)

