For presentation at the Fuel Cell Projects Kickoff Meeting, DOE Headquarters, 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

Sandia National Laboratories

Objectives

and validate a two-phase, three-dimensional transport
imulating 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

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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., Kulikovsky (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)

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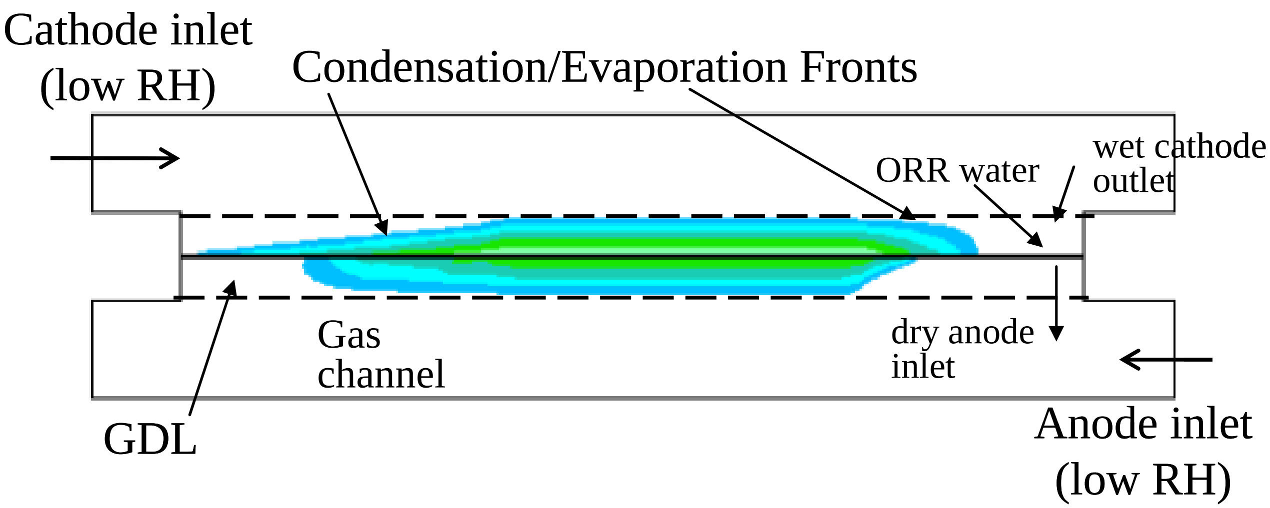
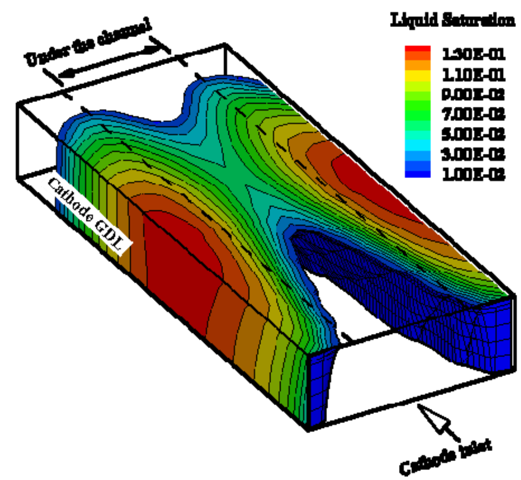
Approach: Develop a unified model and computer code for a wide range of operating conditions (dry, dry-wet, and wet)

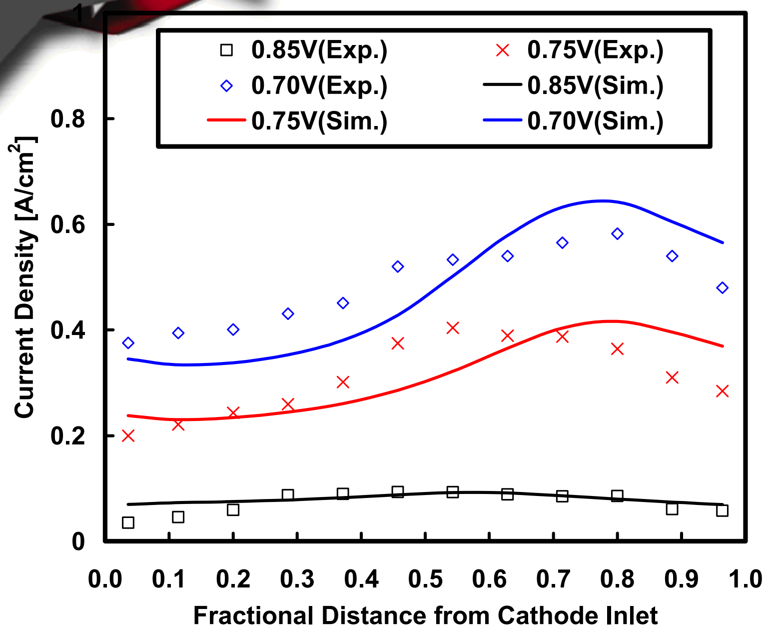


Luo, Ju, and Wang,
J. Electrochem Soc,
154, B316-B321(2007)

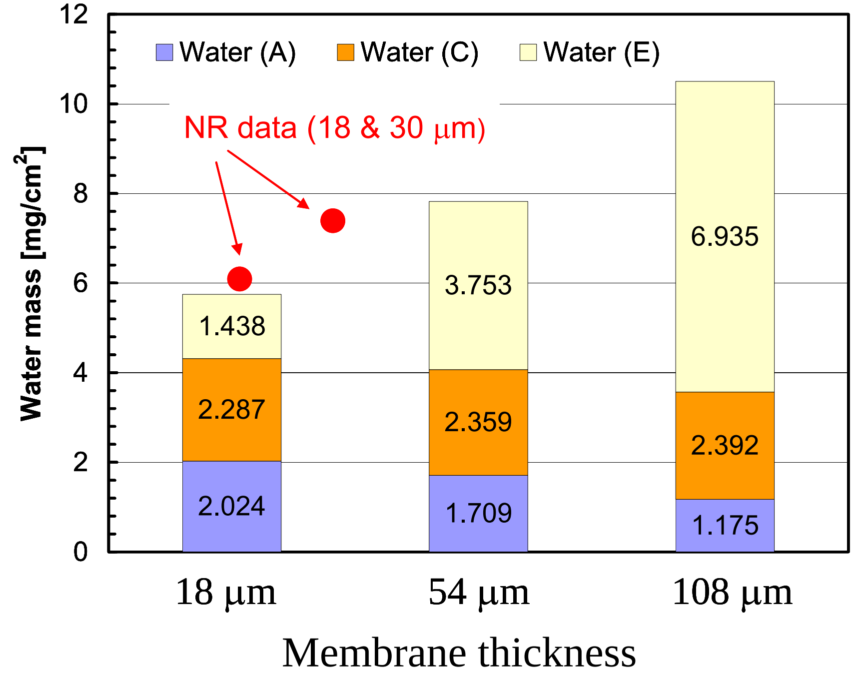
- **Dry-to-wet transition (moving boundary) inside fuel cells is the greatest challenge of water management modeling.**
- **Prior work (Luo et al., JES 2007) developed a basic numerical model for single straight-channel fuel cells.**
- **Developing a comprehensive numerical model for commercial-scale,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

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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

Project timeline and milestones

Task/Milestone	PY1 (FY09-FY10)				PY2 (FY11)				PY3 (FY12)				PY4 (FY13)			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
1.1/Physical & electro- chemical, mathematical, sub-model development												M6				
1.2/Numerical implementation and algorithm development												M7				
1.3/Integrated computer code development and testing				M1 G1				M3 G2				M8 G3				
2.1/Model-input parameter measurements				M2				M4				M9				
2.2/Model-validation data generation				M2				M4				M9				
3.1/Model validation for single-cell model in the partially two-phase regime								M5 G2								
3.2/Model validation for single-cell model in the fully two-phase regime												M10 G3				
3.3/Model validation for short-stack model														M11		
4/Identifying rate-limiting steps and developing recommendations for improvements in automotive applications															M12	
4 /Identifying rate-limiting steps and developing recommendations for improvements in stationary applications															M12	
5.1/Public dissemination of model via publications																M13
5.2/Providing instructions for exercising model																M13
5.3/Compilation of data generated in project																M13

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

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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

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

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

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

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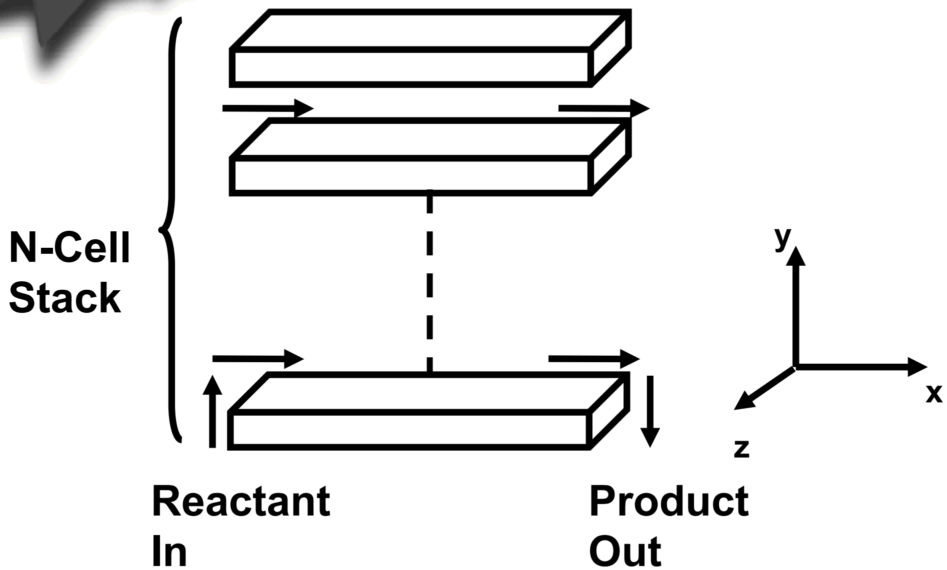
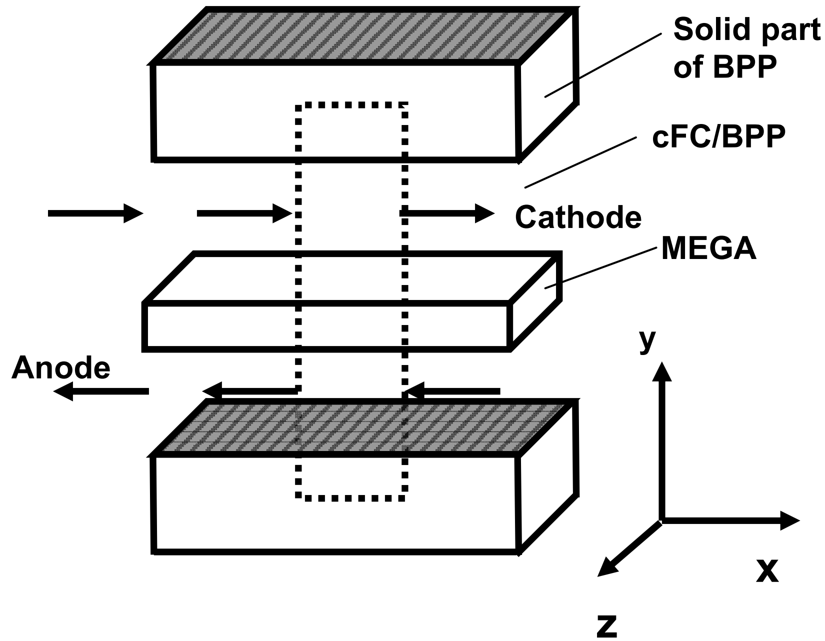
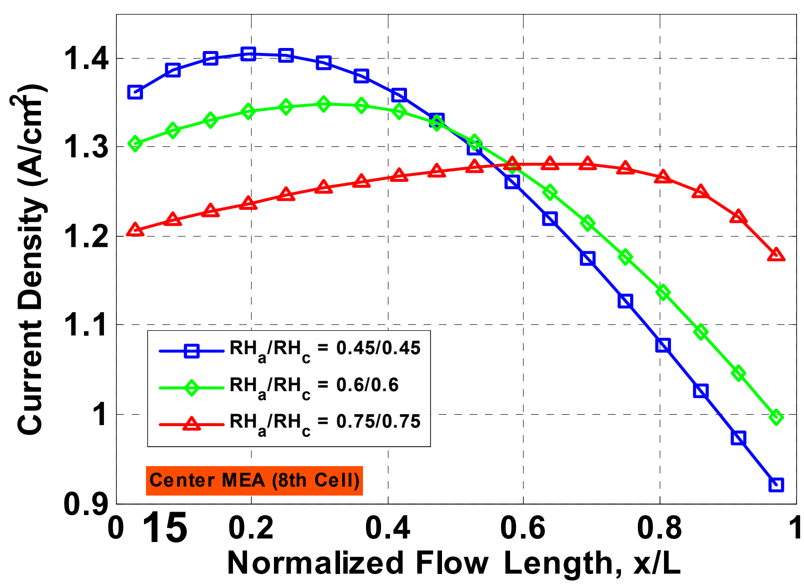
Approach: develop a numerically efficient short stack model





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



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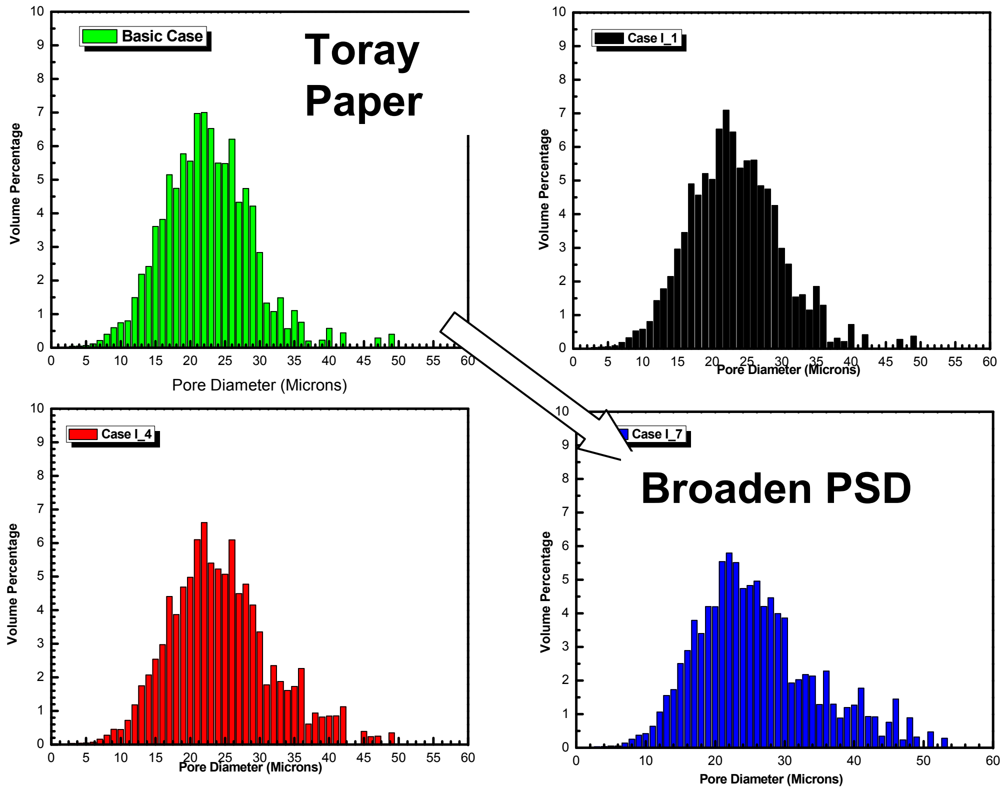
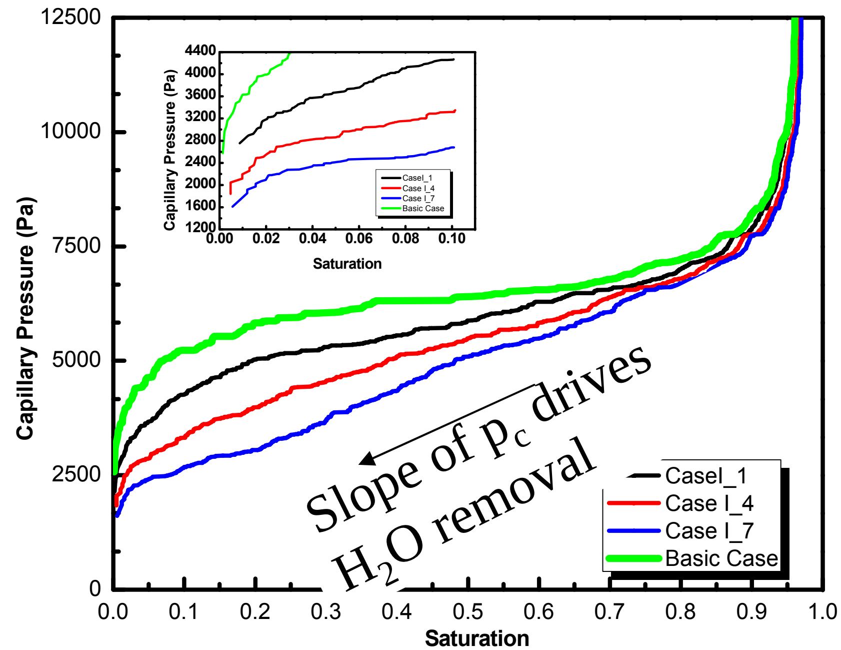
Approach: Address relationships among GDL pore structure, transport properties and cell performance (I)





with different increasing ratios of pore and throat size at GDL inlet

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

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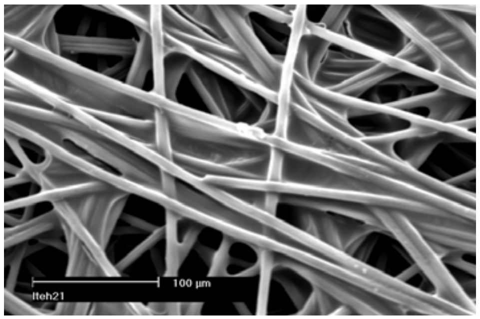
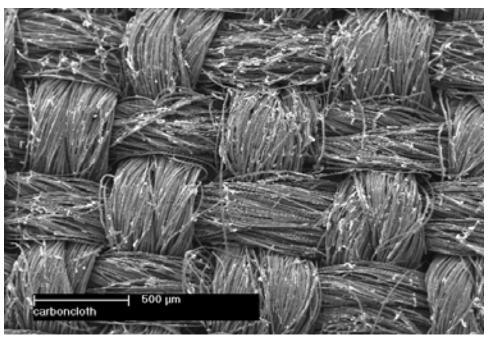
Approach: Address relationships among GDL pore structure, transport properties and cell performance (II)





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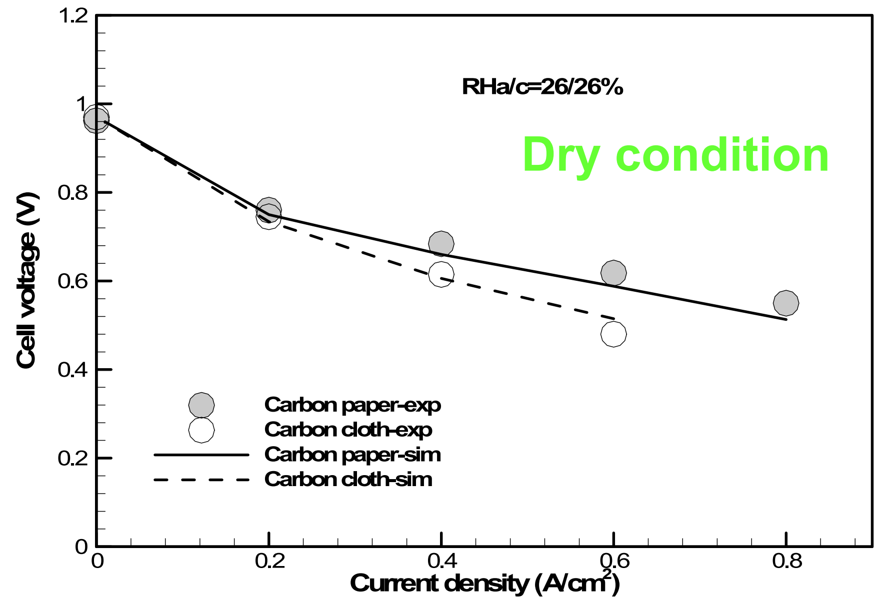

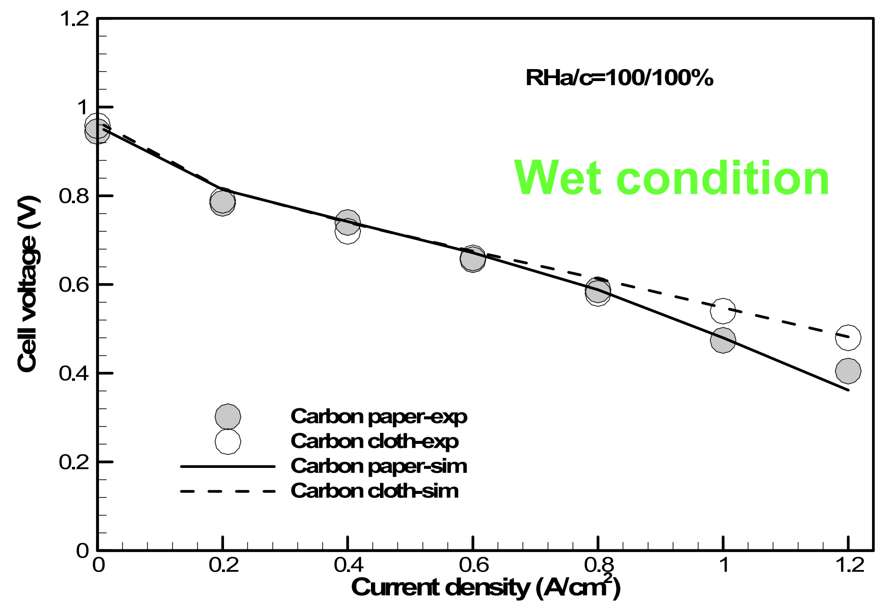

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