SAND 2012-2037C

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

Ken S. Chen (PI)
Brian Carnes
Sandia National Laboratories

May 15, 2012

FC027

Overview

Timeline

- Project start date: 10/1/09
- Project end date: 9/30/12
- Percent complete: ~85%

Budget

- Total project funding (over 3 years)
  - DOE share: $2.246M
  - Contractor share: $238K
- Funding received in FY11: $798K
- Funding for FY12: $400K

Barriers

- Barriers addressed
  - **Performance**
  - **Cost**

The validated PEM fuel cell model can be employed to improve and optimize PEM fuel cells design and operation and thus address these two barriers.

Partners

- Direct collaborations with Industry, University and other National Labs:
  Nissan (no cost), Ballard
  Penn State University
  LANL, LBNL.
- Project lead: Sandia National Labs

Objective/Relevance

Sandia National Laboratories

- The project objective is twofold:

  1) to develop and validate a two-phase, three-dimensional transport model for simulating PEM fuel cell performance;

  2) to apply the validated PEM fuel cell model to improve fundamental understanding of key phenomena involved and to identify performance-limiting phenomena and develop recommendations for improvements so as to address technical barriers and support DOE objectives.

- The coupled DAKOTA/PEMFC model computational capability can be employed to improve and optimize PEM fuel cell design and operation. Consequently, the project helps address the performance and cost technical barriers since improving performance will reduce cost, for example, by using less materials (e.g., catalyst) or minimizing operation cost (e.g., reduce pumping power).

Approach

Our approach is both computational and experimental with active participation from industrial partners:

- Numerically, develop a two-phase, 3-D, transport model for simulating PEM fuel cell performance.
- Experimentally, measure model-input parameters and generate model-validation data.
- Perform model validation using data available from literature and those generated within the team.
- Apply the validated model to identify performance-limiting phenomena and develop recommendations for improvements.

What distinguishes the present work and previous efforts?

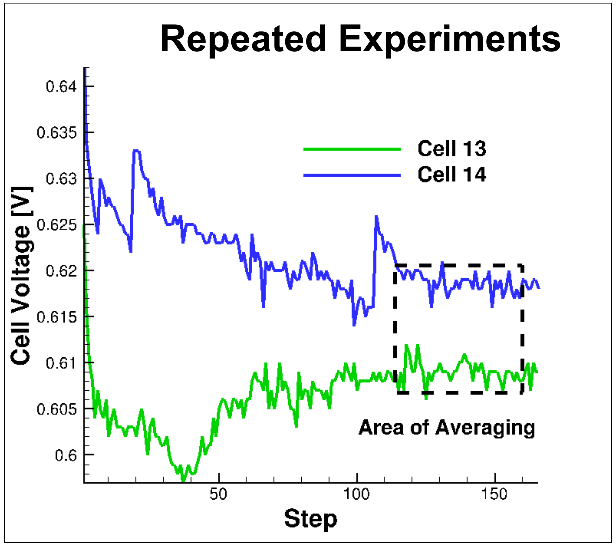
- Couple the PEMFC model with DAKOTA (toolkit for design/optimization) to perform computational DOE (design of experiments) and 3-D detailed probing, sensitivity and variability analyses, and parameter estimation.
- Collaboration with and participation by industry partners, Ballard & Nissan, ensure that the PEMFC model can be used as a practical design tool.

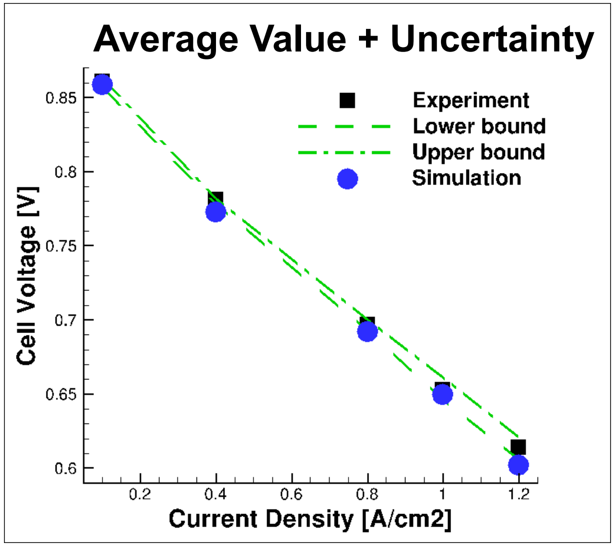
Approach

FY12 Milestones, and Current Status

M/D/Y	Milestone Descriptions	Comments
1/31/12	Perform the validation of the 3-D, partially two-phase, single-cell PEM fuel cell model. Status: completed.	At 80 C validation was acceptable. At 60 C some current over-prediction at high current density (slide 9)
5/31/12	Validate model under real-world conditions and architectures using data from Ballard and Nissan for non-automotive and automotive applications. Goal is to predict experimental current, temperature and cell voltage within 20% or as defined otherwise by Ballard and Nissan. Status: 50% complete.	Nissan collaboration resulted in new sub-models for low Pt loading. Ballard model validation will measure model capability under realistic operating conditions.
7/31/12	Validate fully two-phase, 3-D cell model with microporous layer effect using neutron imaging data. Status: 50% complete.	Direct validation of through-plane liquid water predictions will increase model credibility.
9/30/12	Generate test suite for PEM fuel cell model and create user manual. Status: 25% complete.	These deliverables will enable the model to be run by researchers and industry.

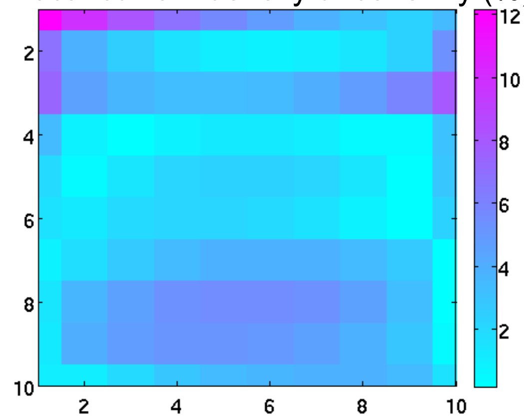
Technical Accomplishment: Uncertainty Quantification of Experiments / Simulations





1.2 A/cm2, 80°C, 100%RH

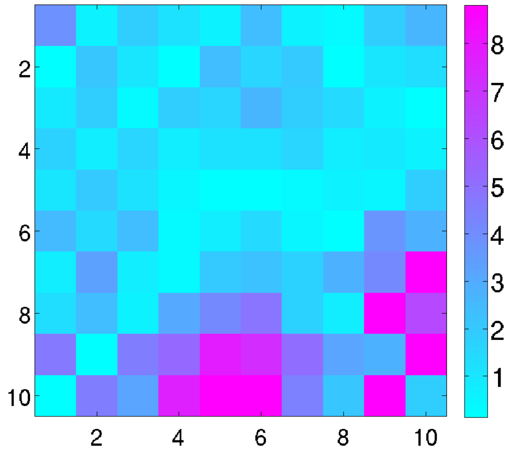
Local current density uncertainty (%)



Repeated experiments (80°C, 100%RH) enables estimation of uncertainty bounds on cell voltage and current density

Uncertainty (percent difference) from numerical errors in computations was also quantified using multiple meshes

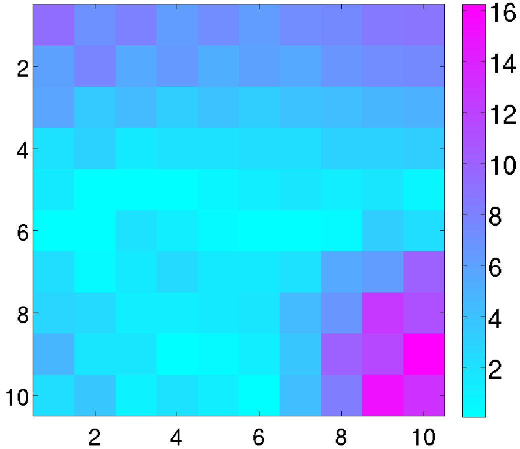
Local current density uncertainty (%)



80 C / 50% RH / 0.1 A/cm2

Uncertainty (variability between repeated experiments) in local quantities like **local current** (10-15%) can be much higher than for integrated quantities like cell voltage (<5%). Numerical uncertainty (error) can be up to 10-15%.

Local current density uncertainty (%)



80 C / 50% RH / 1.0 A/cm2

Technical Accomplishment: Validation of Segmented Cells: Cell Voltage

Operating Conditions: (Co-flow)

I= 0.1, 0.4, 0.8, 1.2 A/cm^2

T_{cell} =60, 80 C , P_a=P_c= 25 psig

Inlet %RH(a/c)= 25, 50, 75, 100

St(a/c) (H_2/air) =1.2/2.0

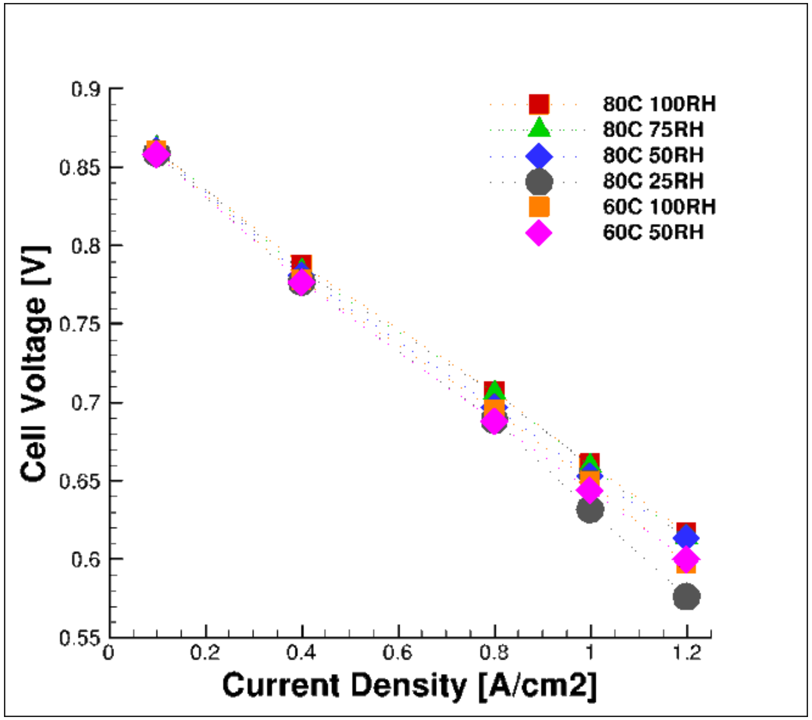
Cell Geometry:

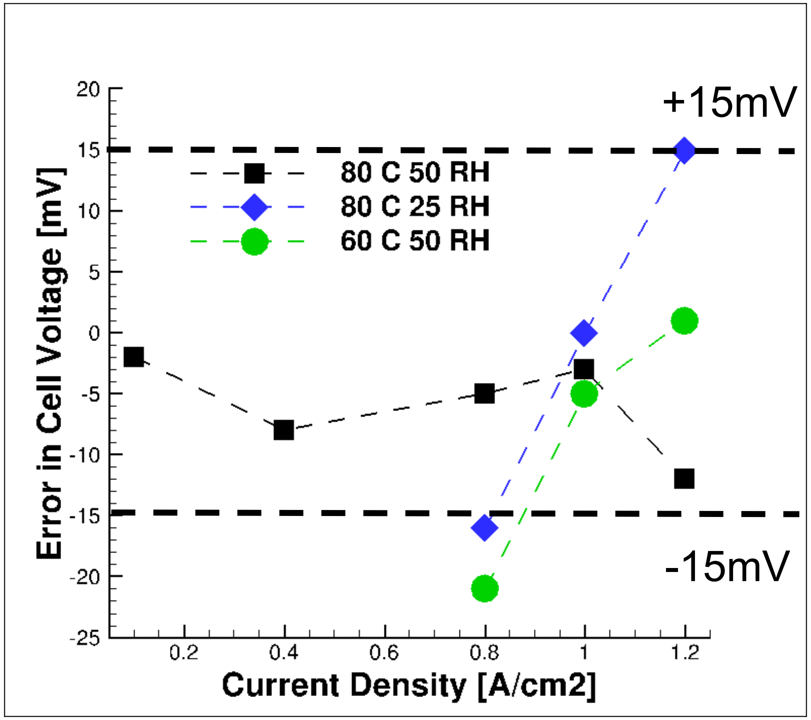
Membrane: 18 um CL(a/c): 7/12 um

MPL: 40 um GDL: 160 um

GFC: 1×1mm Land: 1.1mm

Cell active area: 50 cm^2

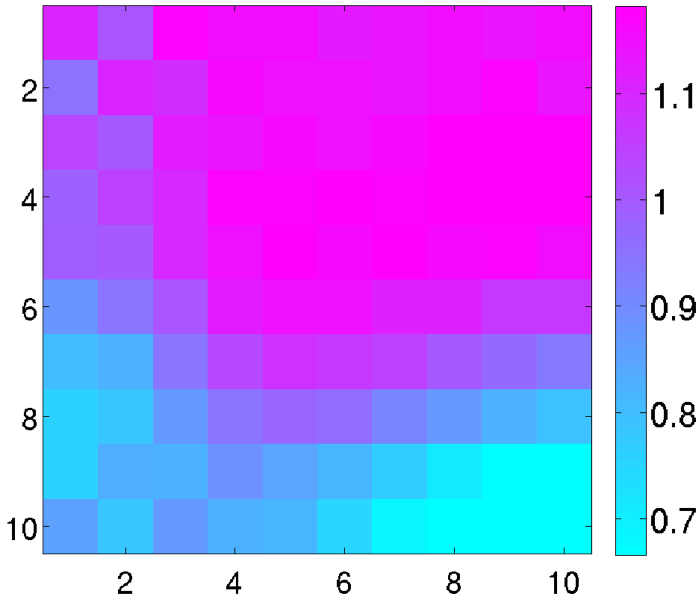




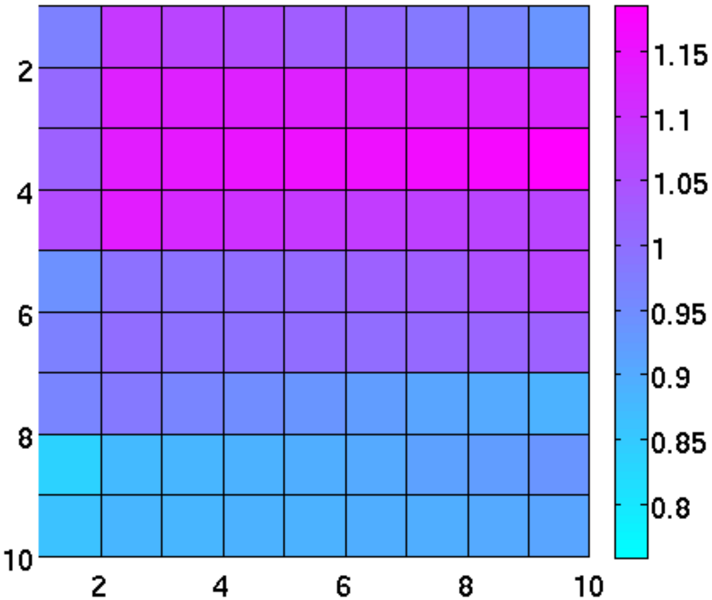
Experimental polarization curves for all 6 operating points. Based on averages of two repeated experiments.

Model validation estimated the cell voltage to within +/-15 mV. Largest errors occurred at high current and at low temperature and relative humidity (RH).

Technical Accomplishment: Qualitative Validation of Segmented Current Density



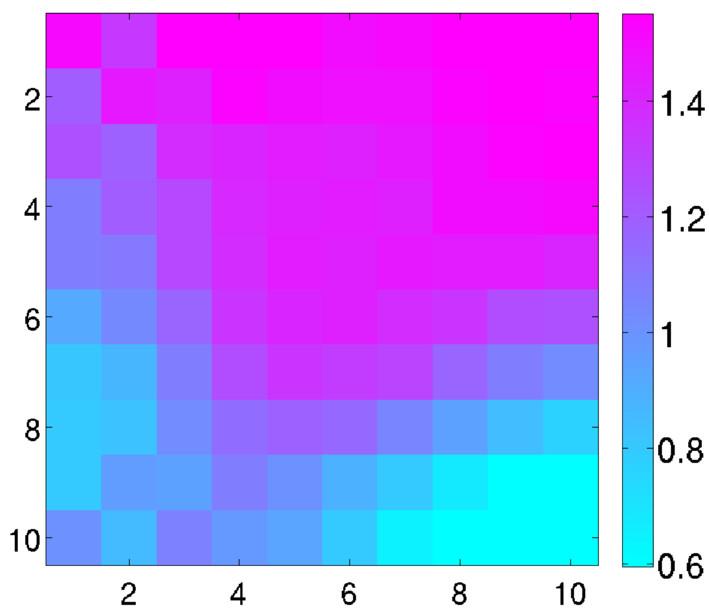
Exp



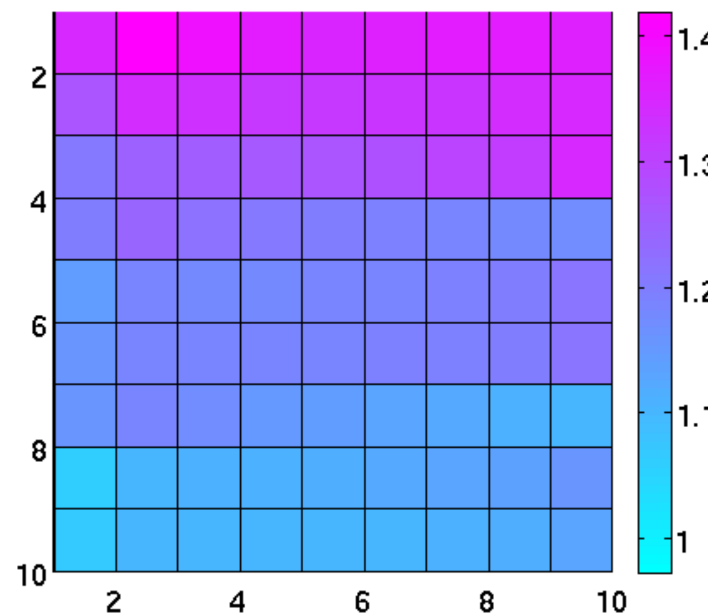
Sim

Comparison of local current density profiles at 80C / 50RH / 1.0 A/cm^2. Note the similar location of the maximum current

Comparison of local current density profiles at 60C / 50RH / 1.2 A/cm^2. Note the similar location of the maximum current

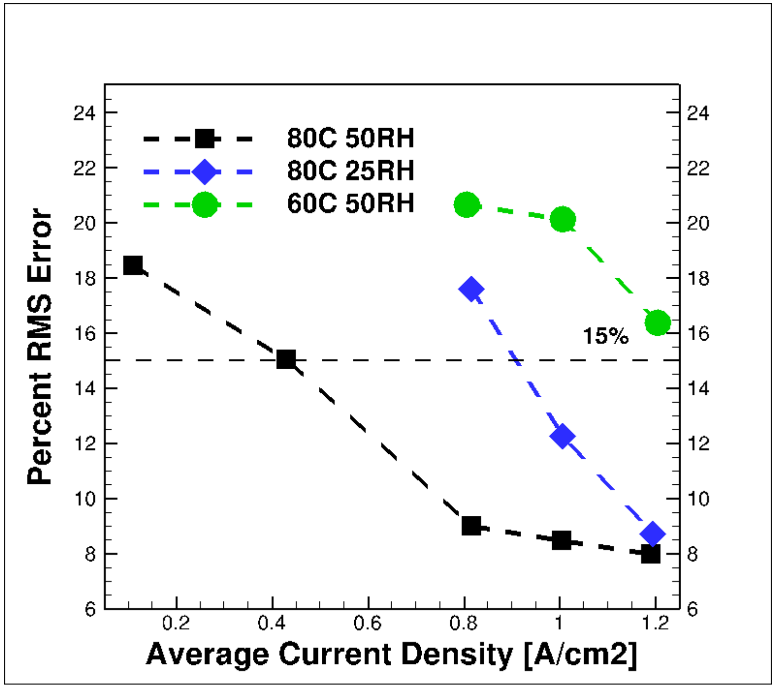


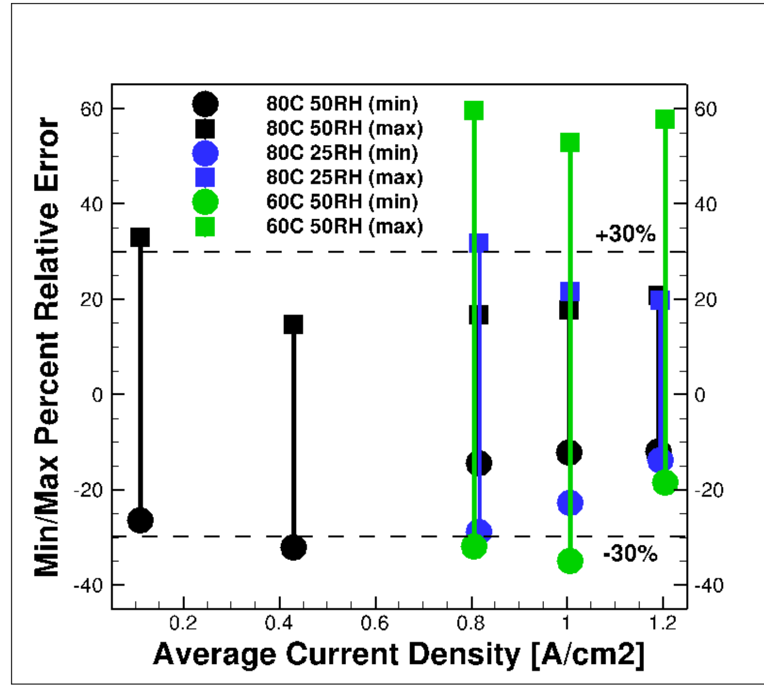
Exp



Sim

Technical Accomplishment: Quantitative Validation of Segmented Current Density





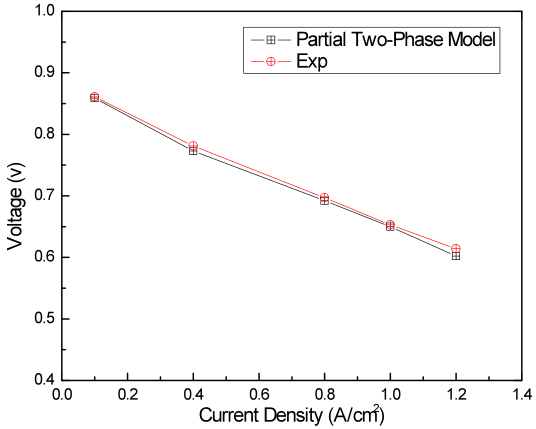
Validation using RMS error in local current density between simulation and experiment at multiple operating conditions.

Validation using min/max local error (5/95 percentile) at multiple operating conditions. This shows the largest local error, with over- or under-prediction indicated by a positive or negative sign.

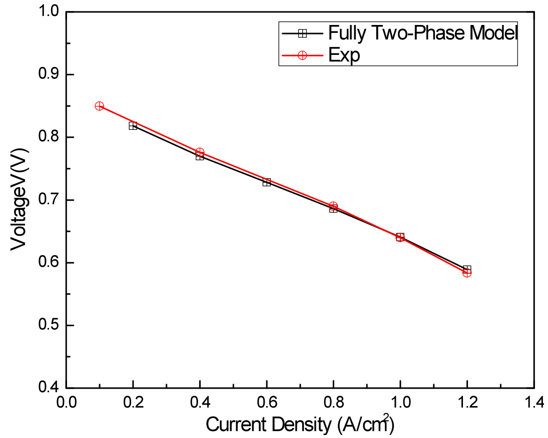
Local current density model predictions were validated at 80C / 50RH and 80C / 25RH (within acceptable bounds). At 60C / 50RH the model may over-predict the local current density. Further work is needed for validation under low temperature operation.

Technical Accomplishment: Comparison Between Partial and Fully Two-Phase Model

Sandia National Laboratories



(a) Partial Two-phase Model



(b) Fully Two-phase Model

Polarization comparison between model predictions and measurement

Operating Conditions:

St(a/c) = 1.2/2.0 (H_2/air)

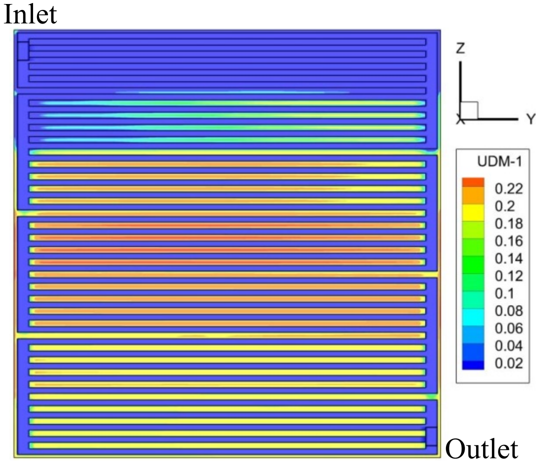
P_a=P_c= 200kPa

T_{cell} =80 °C

Inlet %RH(a/c)= 50.0/50.0

- **Only small difference in polarization prediction between the two models for this 50 cm² cell.**
- **However, the fully two-phase model predicts liquid water in the gas channels comparing to partially two-phase model.**
- **Liquid water predicted by partial two-phase model covers regions only under the bipolar plate.**
- **While liquid water predicted by fully two-phase model appears under both bipolar plate and gas flow channel, especially in the downstream regions near the outlet.**

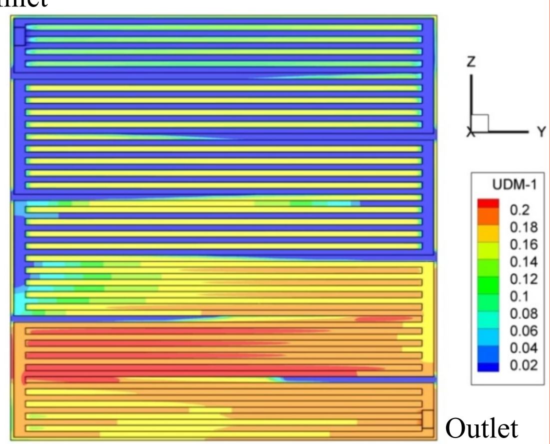
Inlet



Outlet

(a) Partial Two-phase Model

Inlet

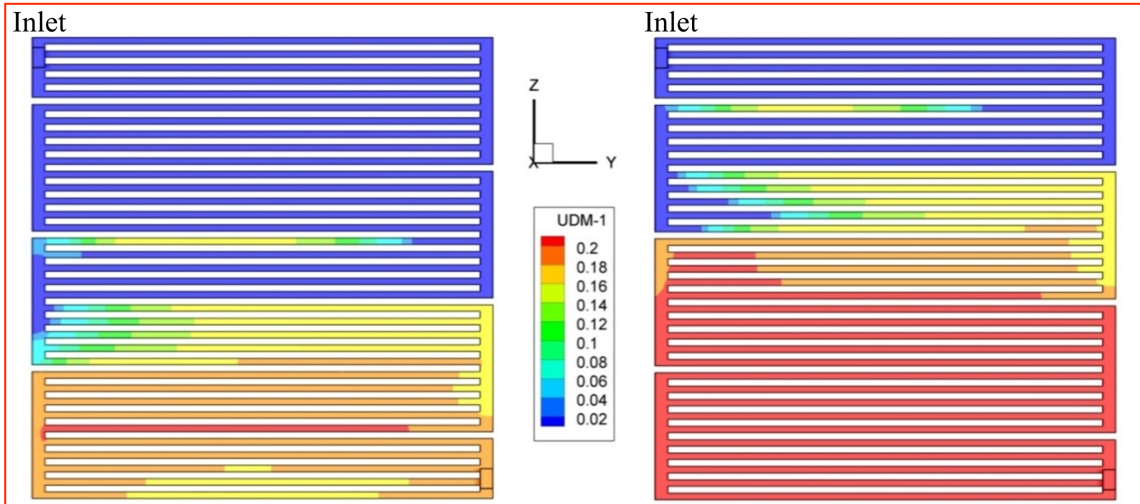


Outlet

(b) Fully Two-phase Model

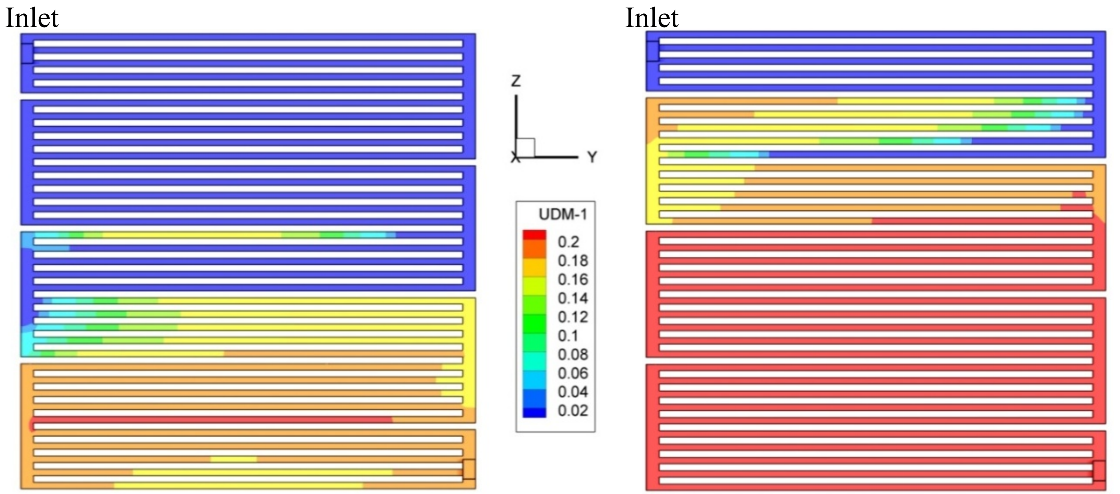
Water saturation distribution at cathode gas flow channel/GDL interface

Technical Accomplishment: Case Study Using Fully Two-Phase Model For Segmented Cell



(a) *RH*=50% Outlet (b) *RH*=72.5% Outlet

Water saturation distribution in cathode GC for different RH



(a) *T*=80 ℃ Outlet (b) *T*=70 ℃ Outlet

Water saturation distribution in cathode GC for different cell temperature

Operating Conditions:

St(a/c) = 1.2/2.0 (H_2/air)

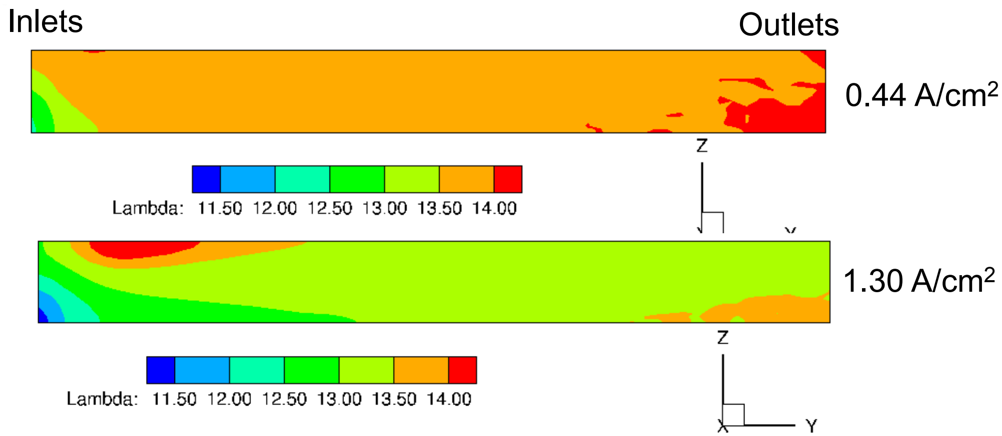
P_a=P_c= 200kPa

CD=0.8A/cm^2

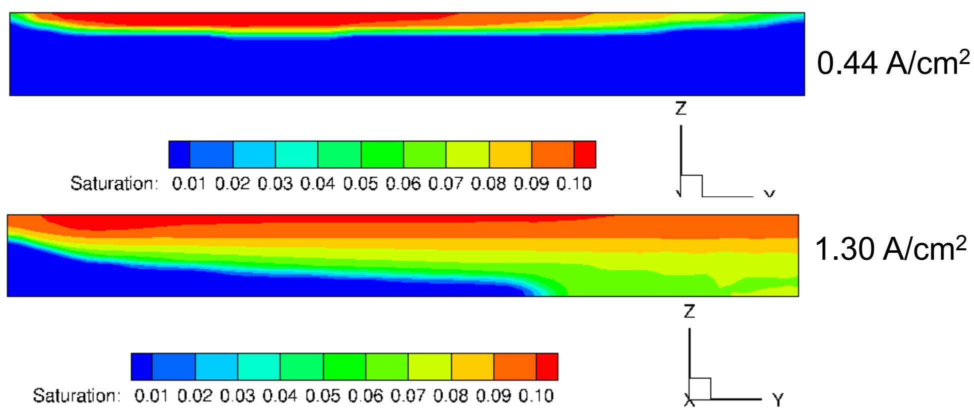
- **More liquid water appears in the gas flow channel with higher inlet relative humidity.**
- **For lower operating temperature, more liquid water is accumulated inside gas flow channels since low temperature are prone to condensation.**

Technical Accomplishment:
Ballard Stack Model (Single Channel)

Sandia National Laboratories



Water content at mid-membrane



Liquid saturation at cathode catalyst layer / micro-porous layer interface

Model can provide local distribution of liquid water for optimal design of flow field and membrane-electrode assembly.

Operating Conditions:
(Co-flow)

I= 0.05-1.30 A/cm^2

T_{cell} =60 C

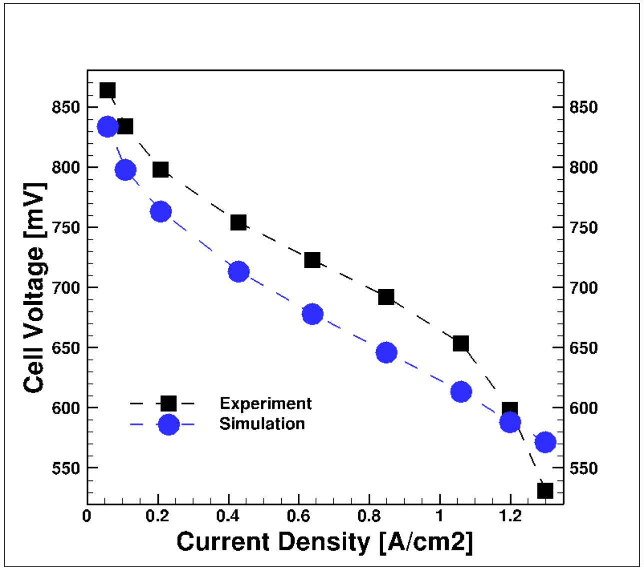
P_a= 1.15-2.18 atm

P_c= 1.99-5.10 atm

Inlet *RH*(a/c)= 95%

St(a) (H_2) = 1.6-6.3

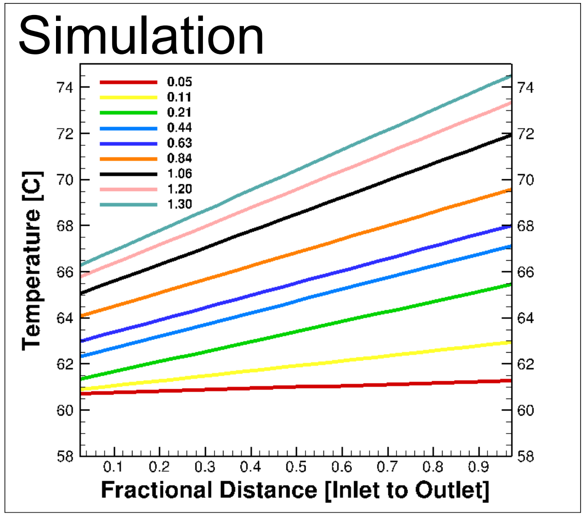
St(c) (air) = 1.8-5.1

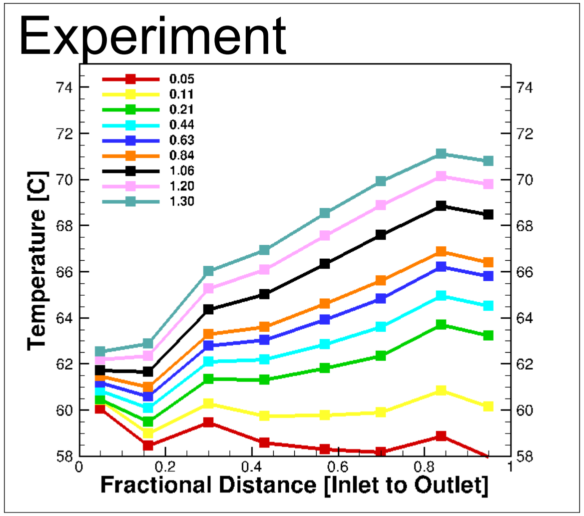


Validation of polarization curve at 60 C / 95% RH

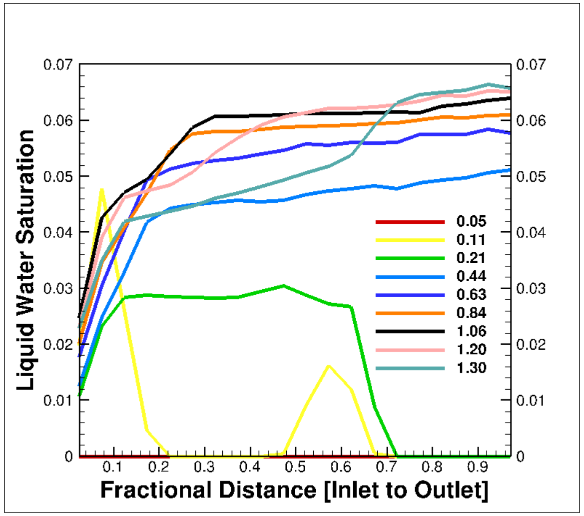
Technical Accomplishment:
Ballard Stack Model (Single Channel)

Validation of average temperature down the channel at various current densities





Simulation of average saturation down the channel (cathode catalyst layer) at various current densities

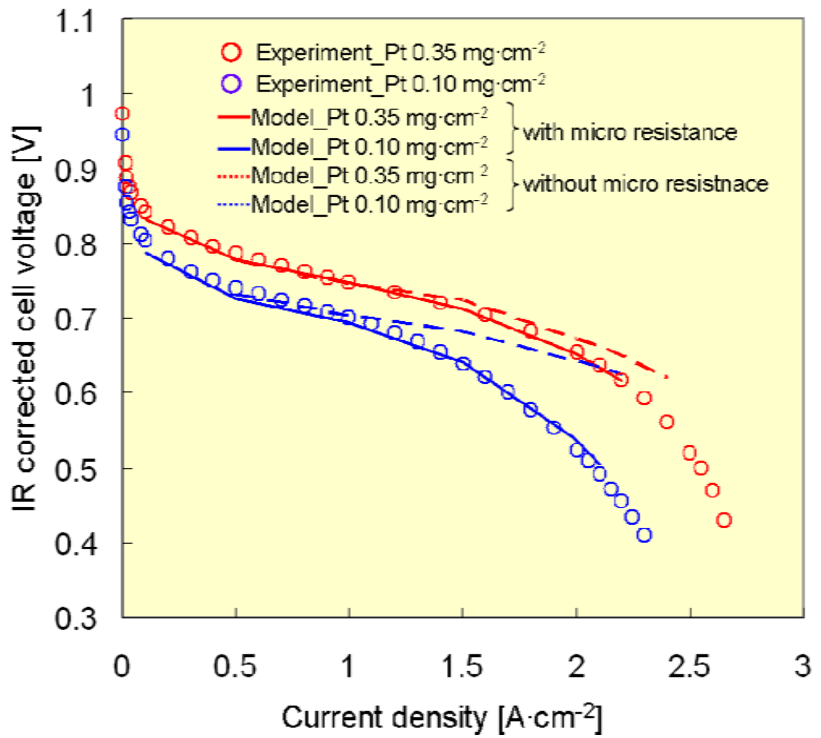


- Current model is complete and being run by Ballard.
- Prediction of main variables (voltage, local current, temperature, and reactants) has been demonstrated.
- Validation of the model predictions for local current, local temperature and polarization is on track for completion this year.
- Model for neutron imaging is currently being built.

Technical Accomplishment:
Nissan Collaboration and Model Validation

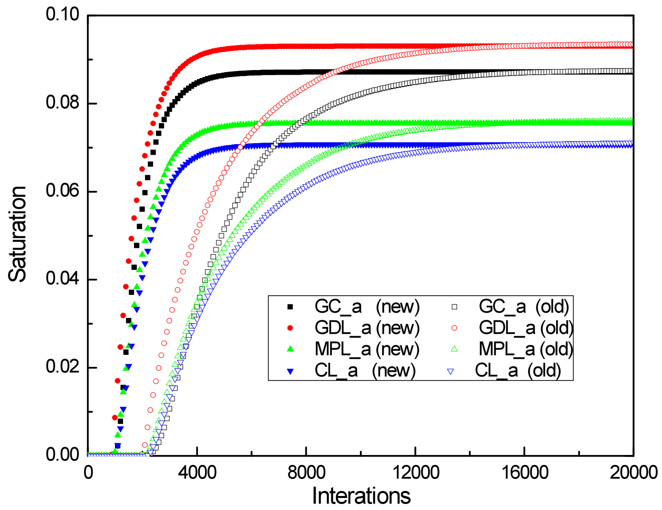
Sandia National Laboratories

- The team is working closely with Nissan to explore the model application to automobiles.
- Nissan sent a visiting scientist to stay at PSU for one year to collaborate on this project.
- Preliminary success has been achieved by Nissan engineers to modify PSU's two-phase code for predicting fuel cell performance with low-Pt loading catalyst layer, as shown in the figure on the right.

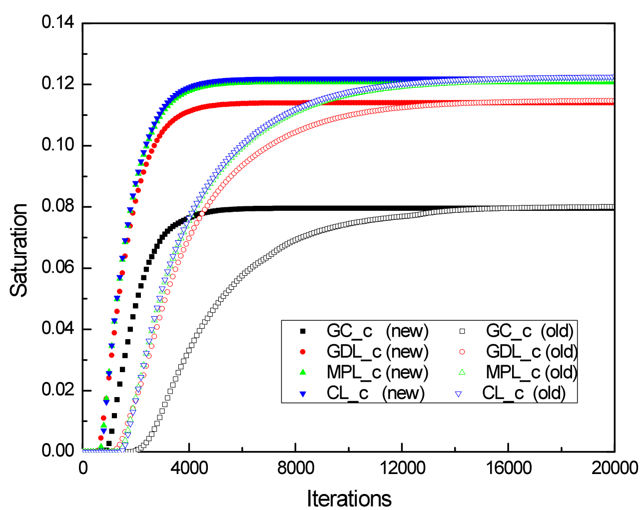


Technical Accomplishment: Improved Convergence for Fully Two-Phase Model

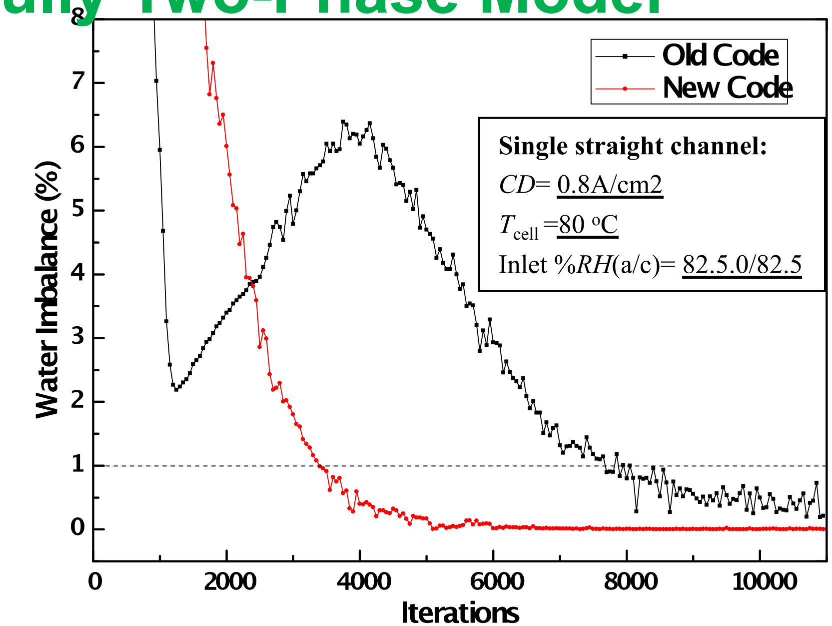
Sandia National Laboratories



Avg. saturation vs. iteration at **Anode side**



Avg. saturation vs. iteration at **Cathode side**



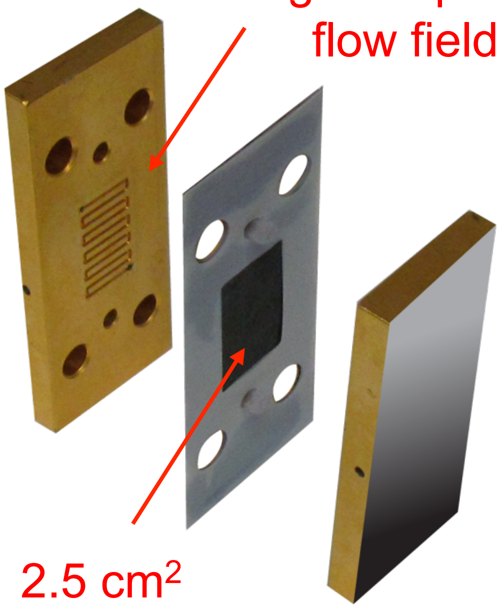
Water Balance for Channel M2 Model

- **Water saturation convergence at both anode and cathode sides is greatly improved for the latest code.**
- **For a typical case, water saturation converges within about 4,000 iterations for latest code, while it needs about 12,000 iterations for previous version. Thus the simulation time is cut by two thirds.**
- **The water imbalance reaches 1% around 3500 iterations for the latest code, while it needs more than 8,000 iterations for previous code.**

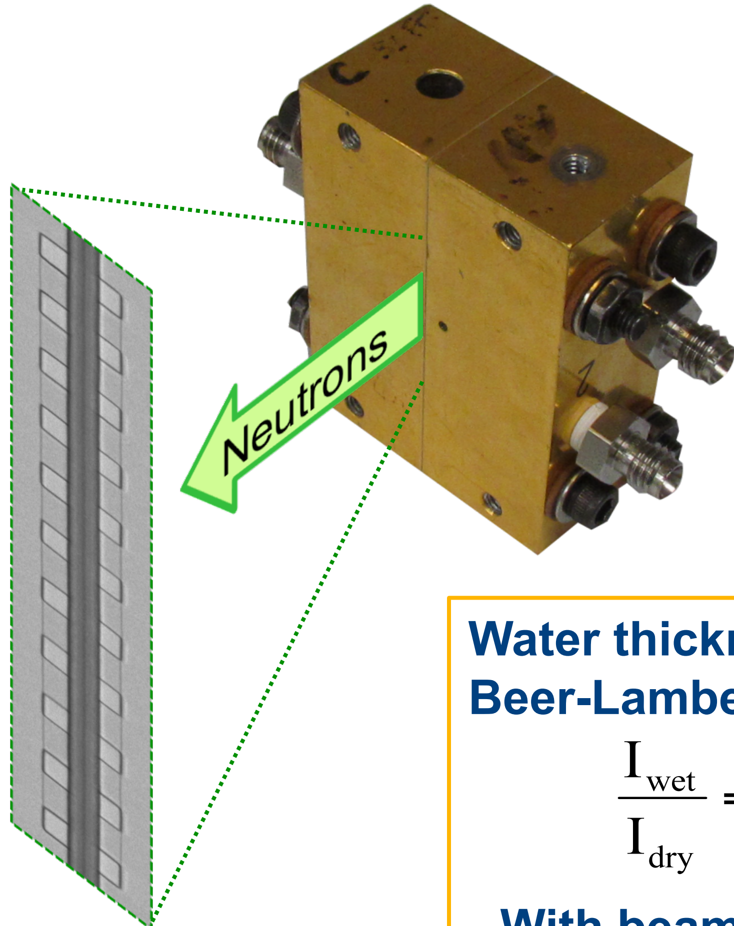
Technical Accomplishment: High-resolution (13 μm) Through-Plane Neutron Imaging

In situ evaluating water content through the thickness.
Varied current density (0.4, 0.8, 1.2 A/cm^2) and RH (50 and 100%)

Single-serpentine flow field



2.5 cm^2 active area, 1.2 cm beam path



Water thickness "t" from Beer-Lambert law:

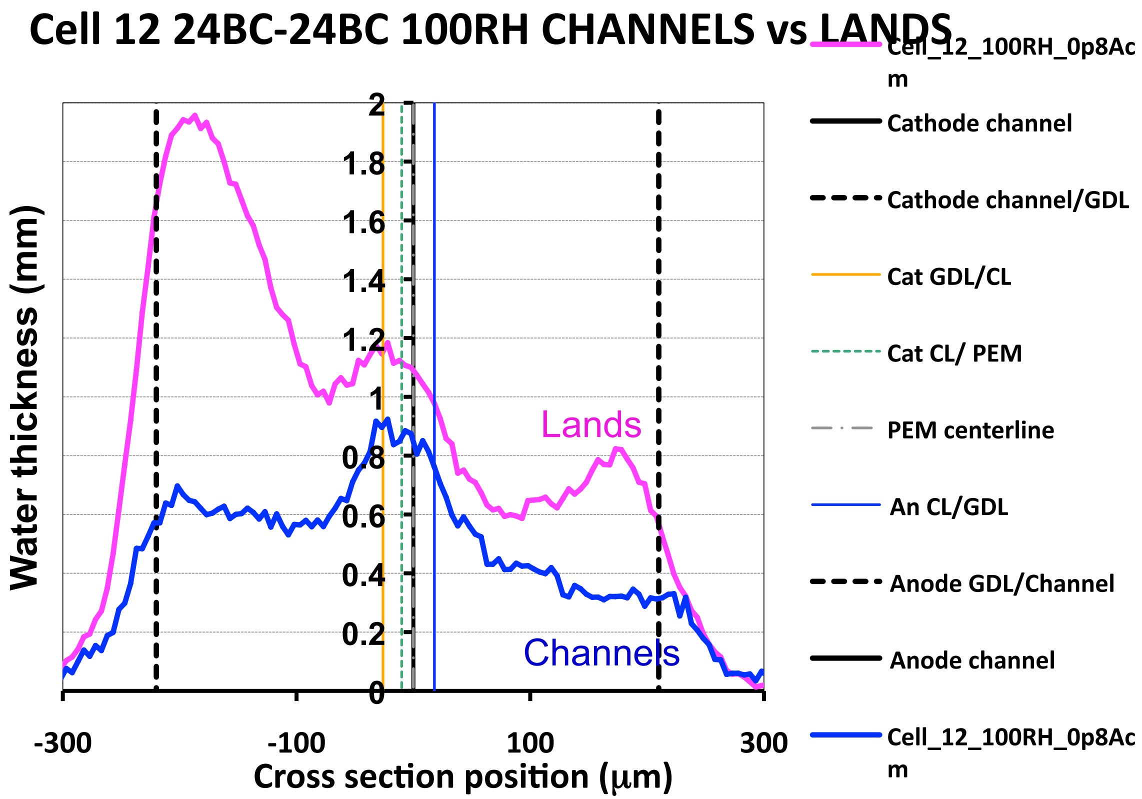
$$\frac{I_{wet}}{I_{dry}} = e^{-\mu t}$$

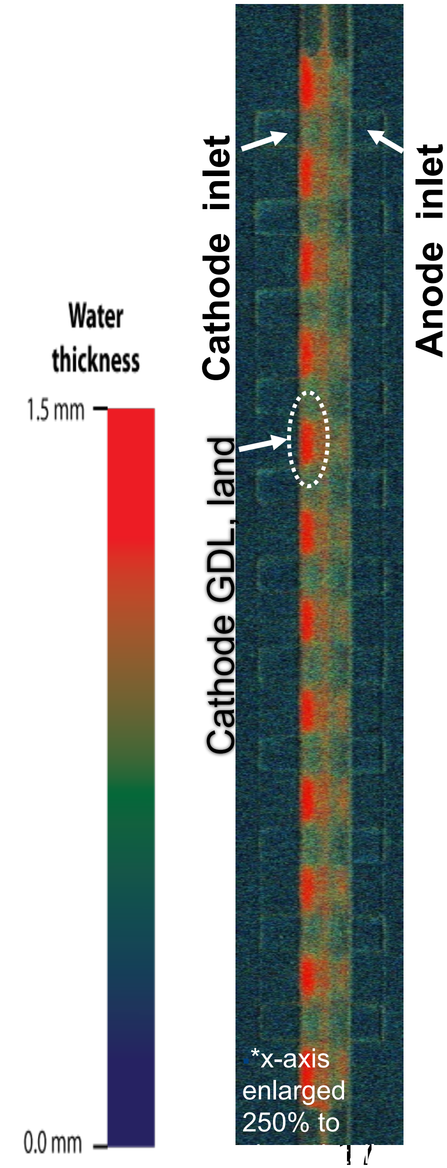
With beam hardening:

$$\frac{I_{wet}}{I_{dry}} = e^{-\mu t - \beta t^2}$$

Technical Accomplishment: High-resolution (13 μm) Through-Plane Neutron Imaging

0.8 A/cm², 80°C, 100%RH

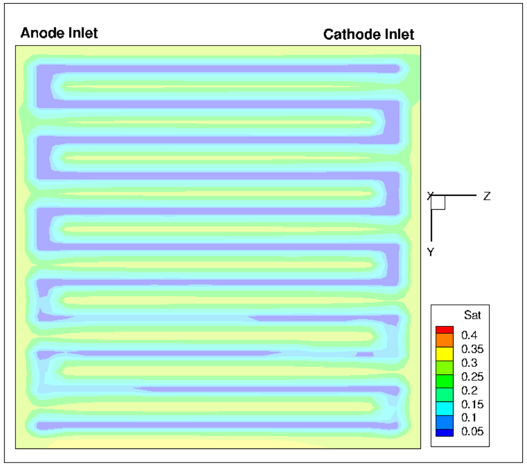




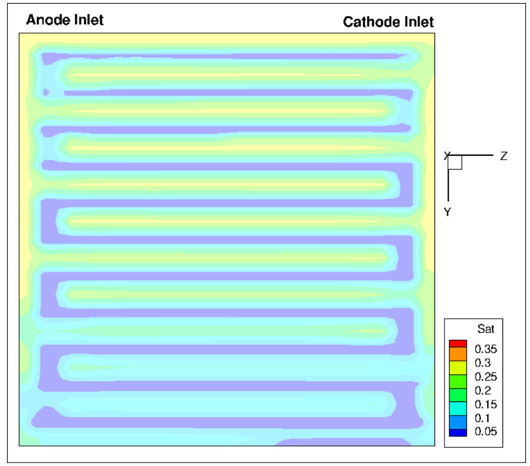
High resolution through-plane liquid water measurements are used for validating predictions of multi-phase models in different layers (GDL/MPL/CH). Separate liquid water data for lands & channels can be directly compared to model predictions.

Work in Progress: Preliminary Validation of Liquid Water Predictions Using Neutron Imaging

Sandia National Laboratories

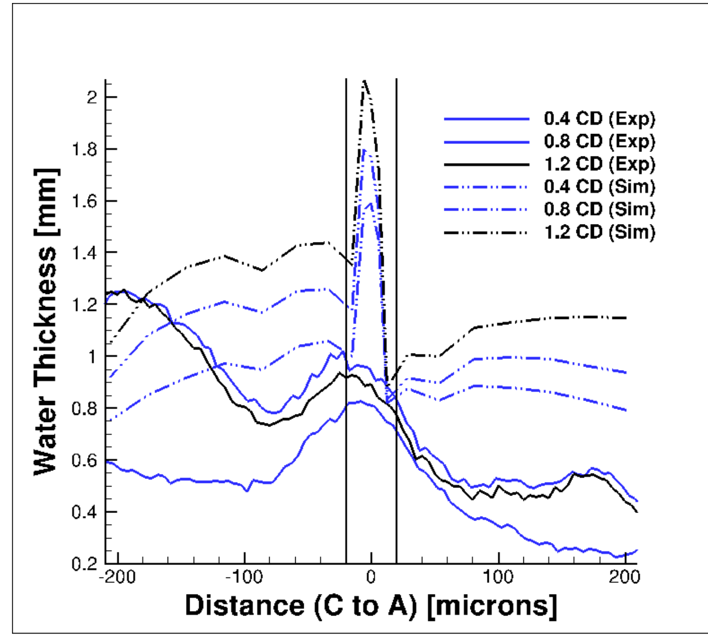


1.2 A/cm^2, 50% RH



1.2 A/cm^2, 100% RH

Liquid water saturation model predictions at Cathode GDL/Channel Interface



Preliminary model validation of water thickness at 100% RH

- **Simulated liquid water saturation was converted to a through-plane water thickness by dividing the cell into small segments (cathode to anode)**
- **The water thickness in each segment was computed by the formula below using saturation (S), cross-sectional area (A), volume (V), porosity (ε):**

$$W = \frac{1}{|A|}\int_V \varepsilon S \, dx$$

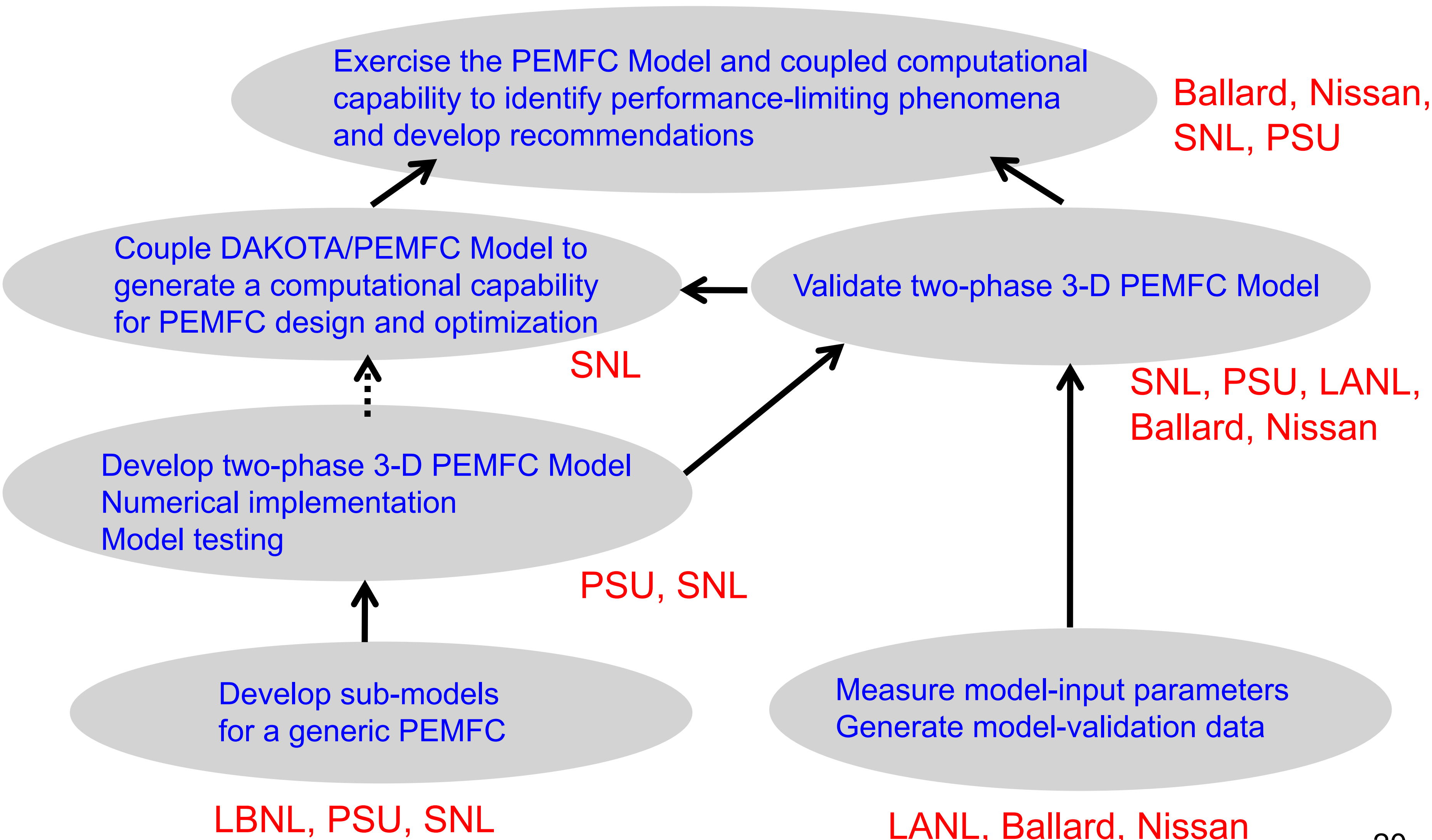
Model validation is on track. We expect to publish a paper this year on model validation using neutron imaging for data measured by LANL at the NIST facility.

Code Dissemination

- A user manual has been documented for the two-phase code we developed over the past decade and further improved in this project.
- The code is currently under testing by project partners, Sandia, Ballard, and Nissan.
- After further development and completion of the project, the software will be made available to the general public under licensing agreements.
- For further information about the two-phase model and computer code, contact Prof. Chao-Yang Wang at cxw31@psu.edu.
- For further information about the DAKOTA interface and scripts, contact Brian Carnes (bcarnes@sandia.gov)

Collaborations

Team partners: SNL(prime), PSU(sub), LBNL(sub), LANL(sub), Ballard(sub), Nissan(no cost)



Future Work

Remaining FY12:

1. Complete model validation in the fully two-phase regimes using neutron imaging data obtained by LANL at NIST
2. Complete validation studies using test data from Nissan and Ballard.
3. Complete code manual and test problems.
4. Submit journal articles on model validation for neutron imaging data.

Summary of Technical Accomplishments

- Model validation using polarization and current distribution data obtained by LANL using a *10*x*10* segmented cell was performed. Year 3 milestone M5 ("Perform validation of the 3-D, partially two-phase, single-cell model") was completed.
- Model validation of liquid water prediction using LANL/NIST neutron imaging data is underway and Year 3 model-validation milestone M3 ("Validate fully two-phase, 3-D cell model … using neutron imaging data") is on track.
- Nissan/Ballard milestone M2("Validate model under real-world conditions") has resulted in model testing under realistic operating conditions.
- Other accomplishments include:
  - Channel liquid water predictions were demonstrated using the fully two-phase model on the LANL 10x10 segmented cell flow field.
  - Demonstration of the two-phase model for predicting liquid water in a form comparable to neutron imaging studies of liquid water for *in situ* fuel cells.
  - A model for micro-resistance was applied for performance prediction of low-Pt loaded catalyst layers for Nissan.
  - Ballard validation of stack data for down-channel current/temp is on track.
  - Validation of Ballard neutron imaging experiments is also on track for completion.

22