SAND2011-1887C

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

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Sandia National Laboratories

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FC027

Overview

Timeline

- Project start date: 10/1/09
  – DOE Kickoff meeting held 9/30-10/1/09
- Project end date: 9/30/13
- Percent complete: ~38%

Budget

- Total project funding (over 4 years)
  – DOE share: $4,292,000
  – Contractor share: $1,200,000
- Funding received in FY10: $232,000
- Funding for FY11: $986,000

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

* PEM refers to polymer electrolyte membrane

Objective/Relevance

- The project objective is twofold:

  1) to develop and validate a two-phase, three-dimensional transport model for simulating PEM fuel cell performance under a wide range of operating conditions;

  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 such as catalyst or membrane or hydrogen fuel or minimizing operation cost (e.g., reduce pumping power).

* PEM refers to polymer electrolyte membrane

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 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 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:
FY10 & FY11 Milestones, and Current Status

Month/Day/Year	Milestone Descriptions
09/30/2010	Develop a three-dimensional, *partially two-phase*, single-cell model and demonstrate model utility in case studies with acceptable numerical convergence measured by absolute residuals of 10^{-5} or less and mass/charge balance error of *2%* or less. Status: completed.
09/30/2010	Measure model-input parameters related to operating cell design (Cell/Component dimensions, Component Physical/Transport Properties, Catalyst Loadings, etc.) and generate model-validation data by measuring Performance Polarization Curves, HFR and AC Impedance for single cells operating at *100%* RH and *50%* RH. Status: completed.
03/31/2011	Measure*10*x*10* current distribution performance data for model validation for 4 different operating conditions (RH = *25%*, *50%*, *75%* and *100%*). Status: completed.
06/30/2011	Develop a three-dimensional, *fully two-phase*, single-cell model and demonstrate model utility in case studies with acceptable numerical convergence measured by absolute residuals of 10^{-5} or less and mass/charge balance error of *2%* or less. Status: near completion.
09/30/2011	Perform validation of the 3-D, partially two-phase, single cell model by comparing computed and measured polarization curves, and current distributions with reasonable agreement (errors fall into the *99%* confidence interval or within +/-*15%*). Status: on track.

Technical accomplishment: Demonstration of fully two-phase PEMFC model – effect of stoich

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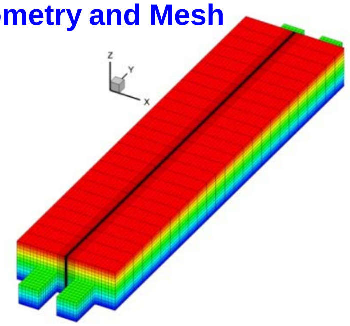
Geometry and Mesh



Cell Geometry:

Membrane: 30 um CL(a/c): 10/10 um MPL: 40 um GDL: 160 um GFC: 1×0.5mm Land: 0.5mm

Cell length (*y* direction): 0.1 m Cell height (*z* direction): 2.0 mm

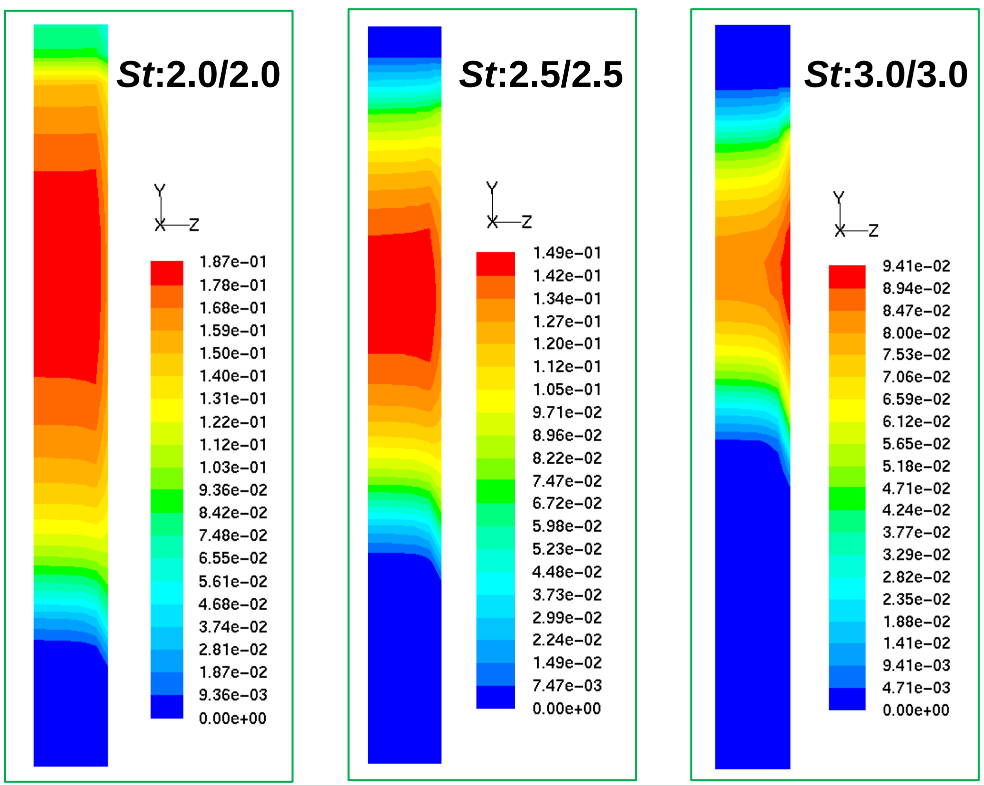
Operating Conditions: (Counter flow)

I= 0.2 A/cm^2 T_{cell} =80 ºC P_a=P_c= 200kPa

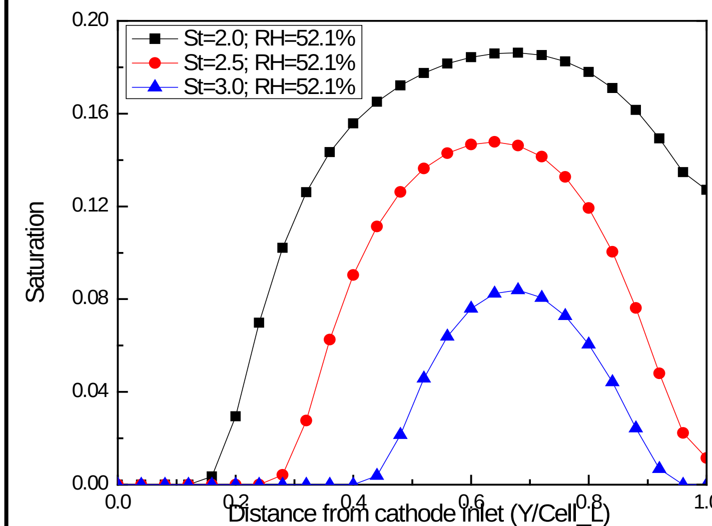
Inlet %*RH*(a/c)= 52.1/52.1

St(a/c) (H_2/air) =2.0/2.0 ; 2.5/2.5 ; 3.0/3.0

Liquid saturation at cathode GFC/GDL interface



Liquid saturation along cathode channel with different stoichiometric flow ratio



❖ **Liquid saturation at the cathode GFC/GDL interface and along gas flow channel decreases with increasing *stoichiometric flow ratio!***

Technical accomplishment: Demonstration of fully two-phase PEMFC model – effect of inlet RH

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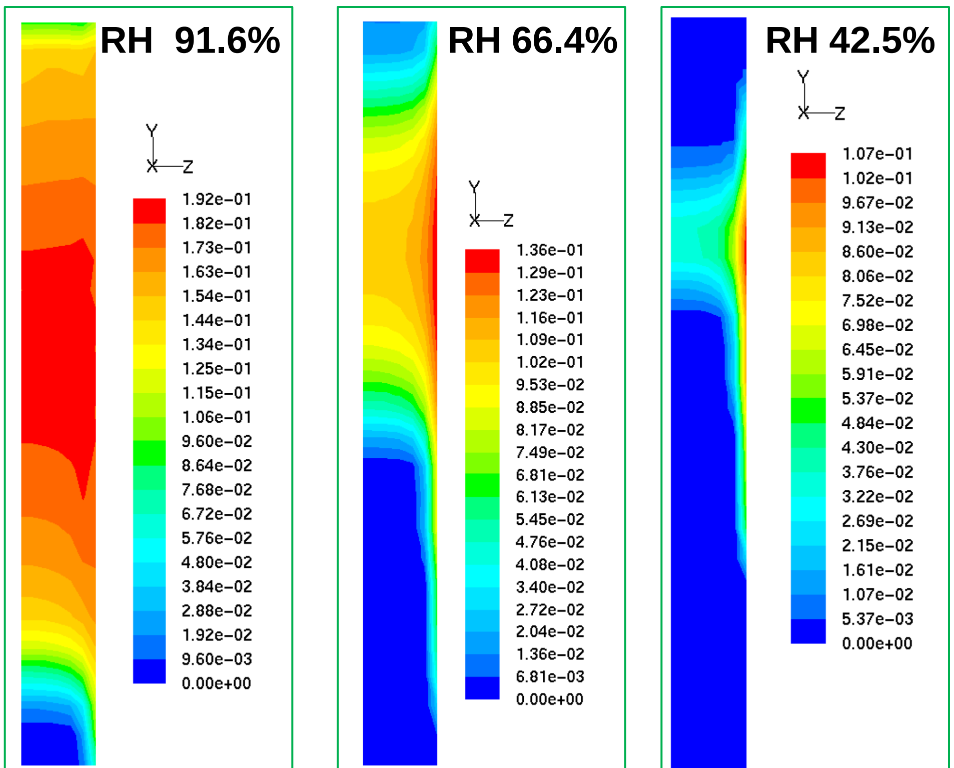
Operating Conditions: (Counter flow)

I= 0.8 A/cm^2 T_{cell} =80 ºC P_a=P_c= 200kPa

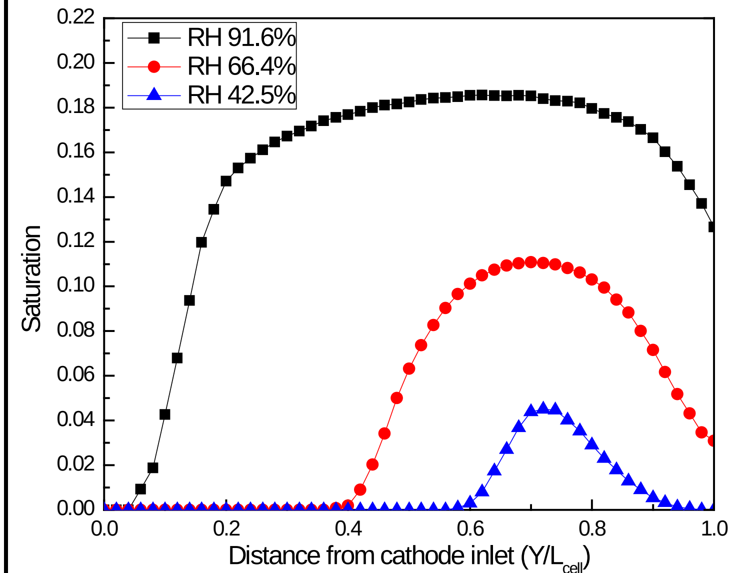
St(a/c) (H_2/air) = 1.8/2.0

Inlet %RH(a/c)= 91.6/91.6 ; 66.4/66.4 ; 42.5 /42.5

Liquid saturation at cathode GFC/GDL interface



Liquid saturation along cathode channel with different anode and cathode RH



- More liquid water is accumulated in the cathode gas channel as anode/cathode inlet RH is raised.
- Liquid saturation near cathode outlet increases with increasing inlet RH, indicating that water transport from cathode to anode decreases.

Technical accomplishment: Demonstration of fully two-phase PEMFC model – effect of current density

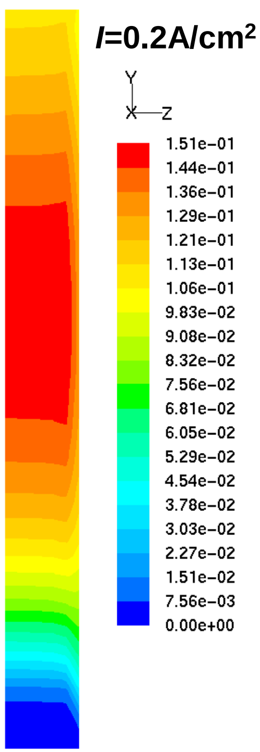
Operating Conditions: (Counter flow)

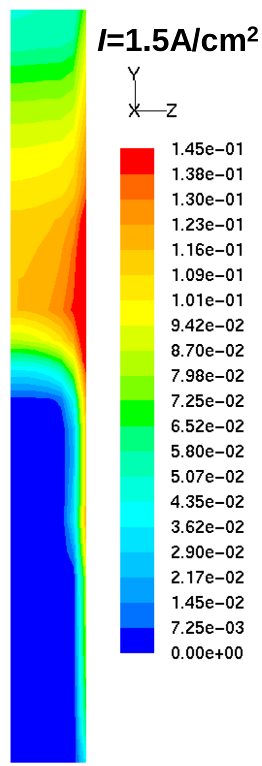
Inlet %*RH*(a/c)= 66.4/66.4 T_{cell} =80 °C

P_a=P_c= 200kPa   *St*(a/c) (H_2/air) = 1.8/2.0

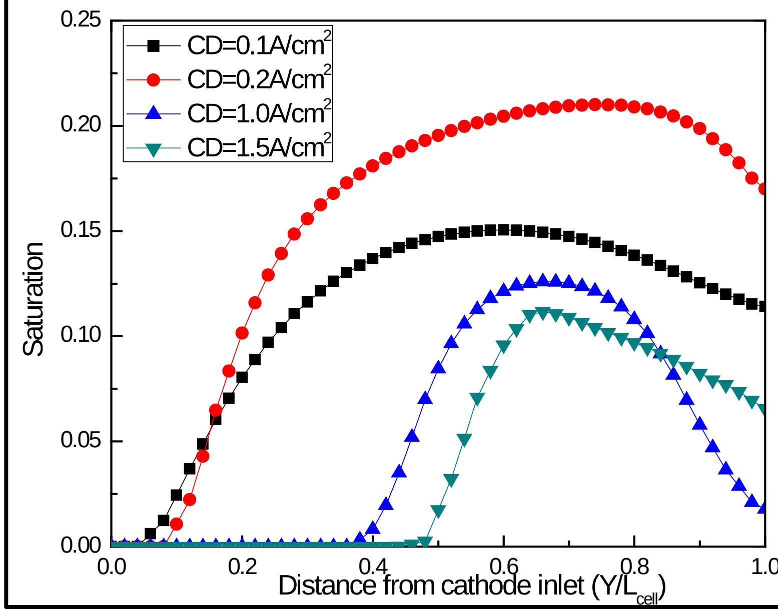
I= 0.1 A/cm²; 0.2A/cm²; 1.0A/cm²; 1.5 A/cm²

Liquid saturation at cathode GFC/GDL interface





Liquid saturation along cathode channel with various current densities



- Cathode gas channel has more liquid water at low current densities than at high current densities – this most likely is due to that sufficiently large drag force is required to remove liquid water from the channel.
- Cathode gas channel has the most liquid water at current density of 0.2 A/cm² for the four cases studied.
- As current density is reduced, the wet region in the cathode gas channel enlarges gradually in both downstream and upstream direction, due to the smaller drag force of gas flow.

Technical accomplishment: Demonstration of fully two-phase model – PEMFC with Chevron flowfield

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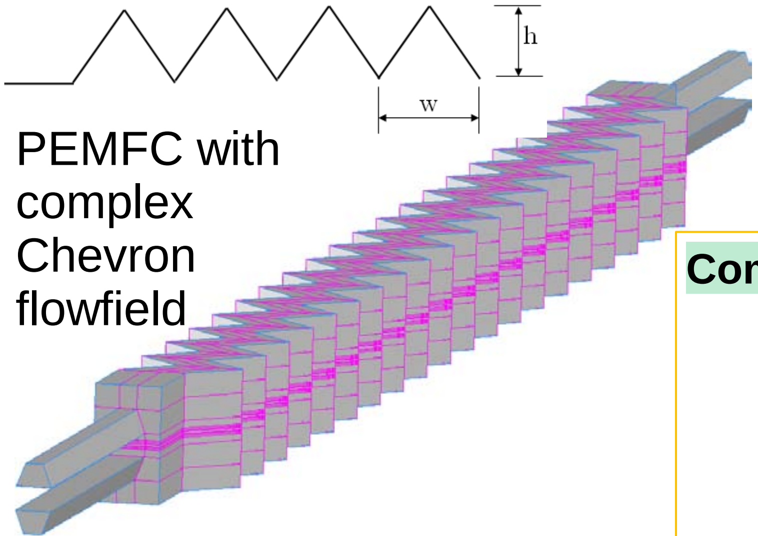


PEMFC with complex Chevron flowfield

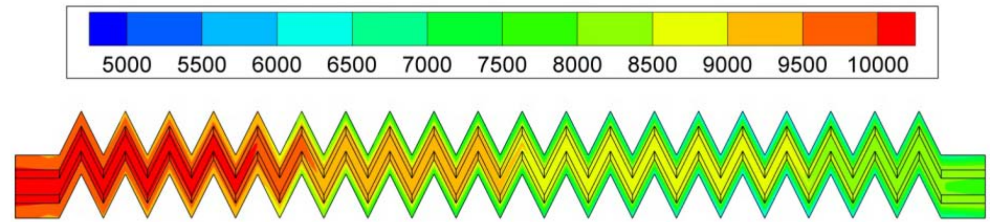
Operating Conditions and geometry (Counter flow)

I= 1 A/cm^2 St(a/c) = 2.0/2.0 (H_2/air) T_{cell} = 80 °C

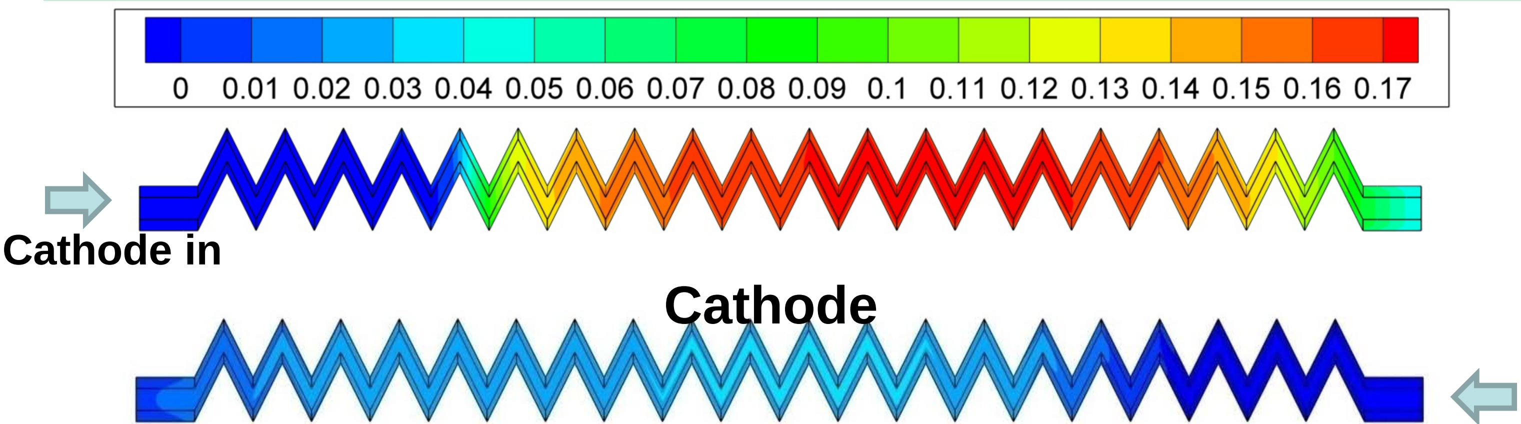
P_a=P_c= 200 kPa Inlet %RH(a/c)= 81.4/81.4

w= 5 mm, h= 1 mm, Membrane: 50 μm, GDL: 150 μm

Computed current density at mid-plane of membrane (A/m^2)

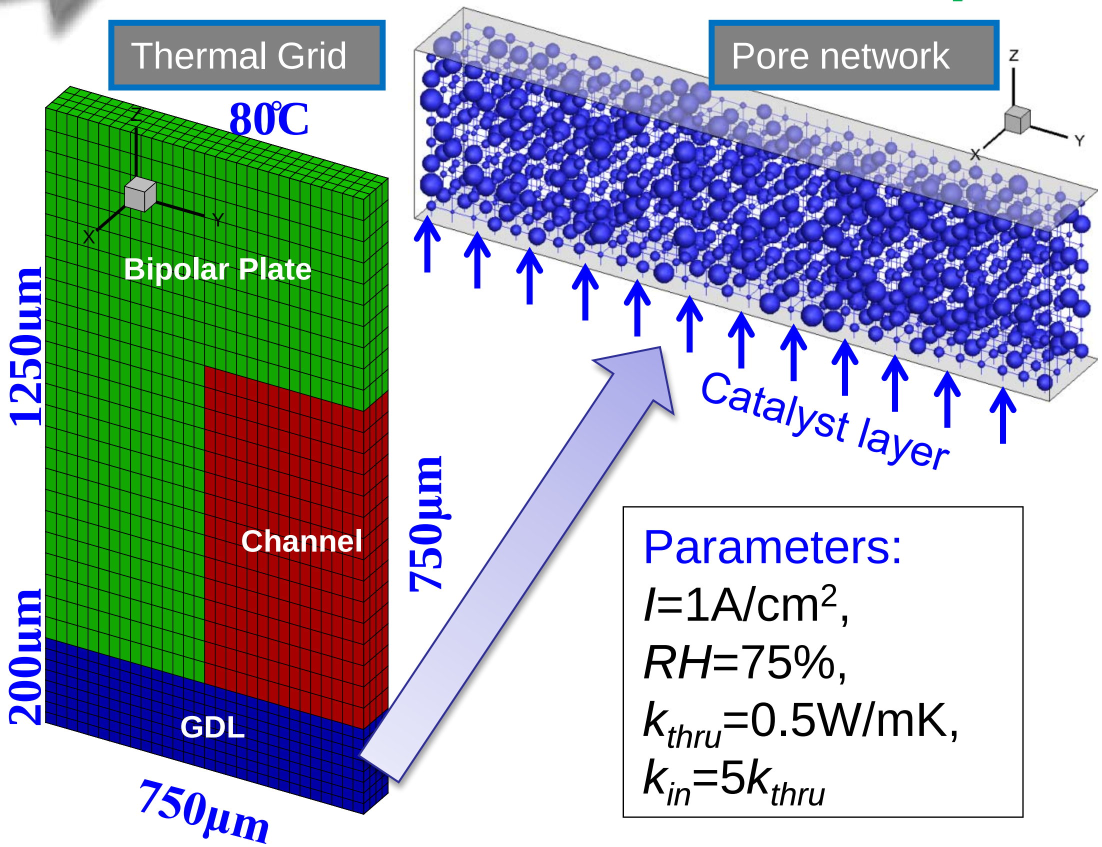


Computed liquid-water saturation along gas flow channel

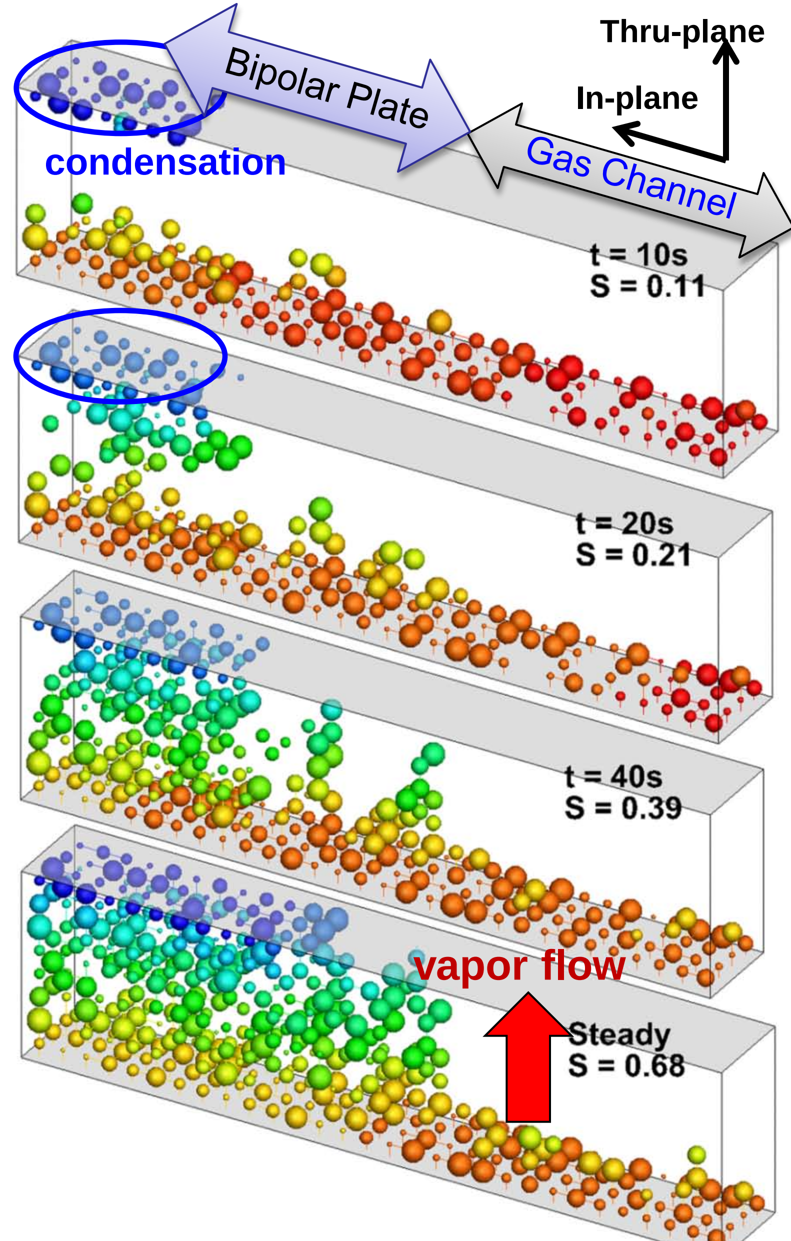


- **The present model is capable of simulating PEMFC with complex flowfield!**

Technical accomplishment:
Nonisothermal pore network modeling: Saturation and temperature evolution



Parameters:
I=1A/cm^2,
RH=75%,
k_{thru}=0.5W/mK,
k_{in}=5k_{thru}



Model Capabilities:
- Heat transfer in pores & solid matrix
- Water vapor diffusion in the pores
- Phase change rates (diffusion limited) & location
- Capillary dominated drainage (invasion & condensation)
- Capillary dominated imbibition (evaporation)

Technical accomplishment: 3-D CFD verification of simplified analytical model for predicting water-droplet detachment

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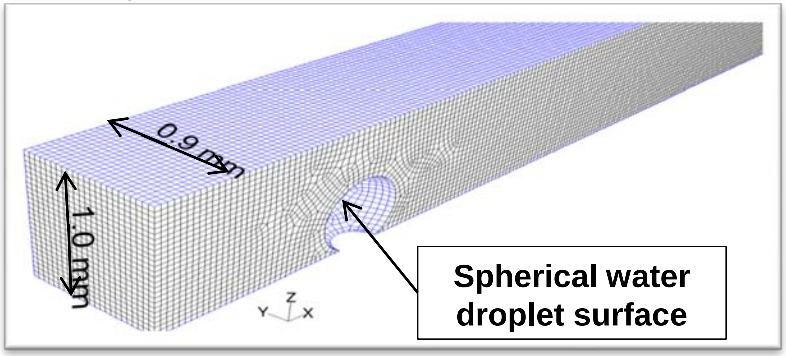
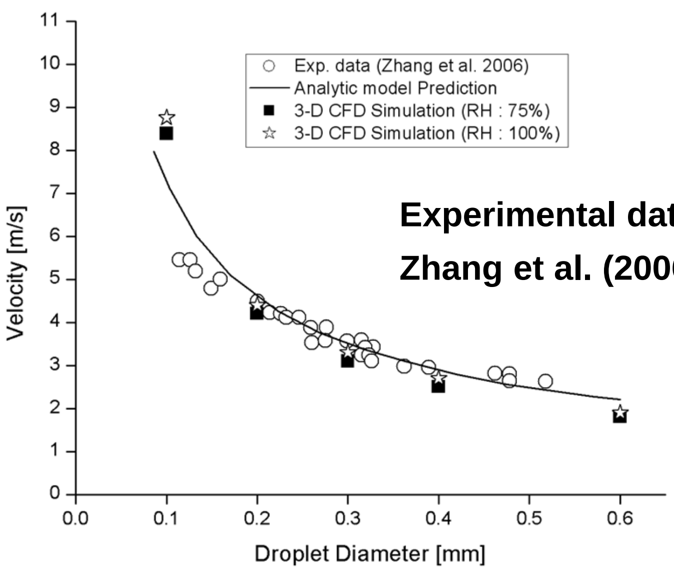
Model geometry for 3-D CFD simulation

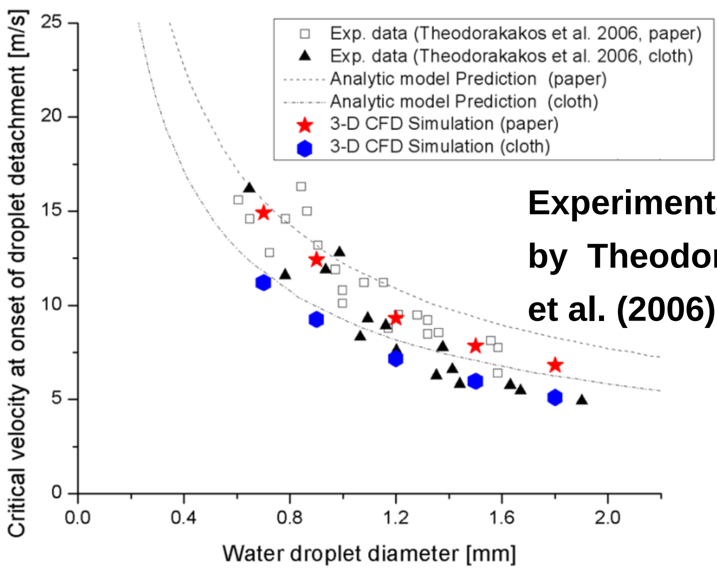


Analytical model: detachment velocity as a function of droplet size (Chen 2008)

$$V_c = \left[\frac{H_c}{\rho\mu}\right]^{1/3}\left[\frac{\pi\gamma \sin^2\theta_s \sin\frac{1}{2}(\theta_a-\theta_r)}{5(\theta_s - \sin\theta_s\cos\theta_s)d}\right]^{2/3}$$

3-D CFD verification and experimental validation of analytical droplet-detachment model



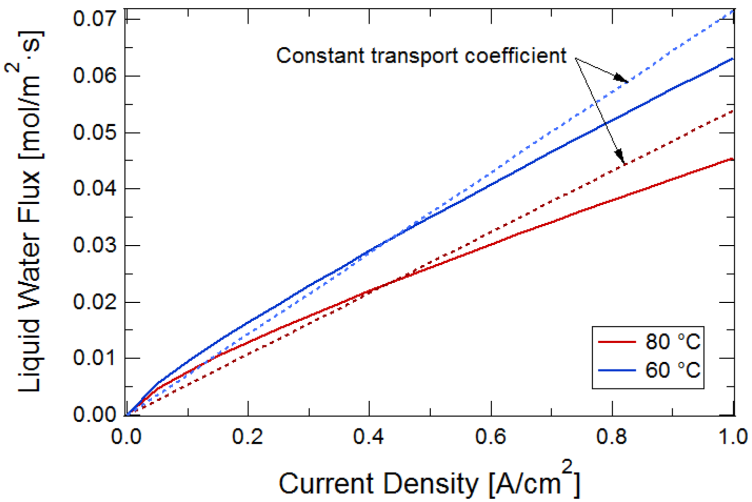


- Agreements between analytical model prediction, 3-D CFD simulation, and experimental data are reasonably good!

Technical accomplishment:

Estimating Liquid Water Flux at GDL/channel interface

1. Calculate the critical pore radius based on force balance
2. Calculate the liquid-water flux out of the GDL/channel interface:



3. Integrate GDL pore-size distribution to obtain number of pores of each size at the GDL/channel interface
4. Determine flow rate through each pore size (assume largest to smallest in terms of filling)
5. Correlate droplet growth and detachment with the liquid water flux and flow rate

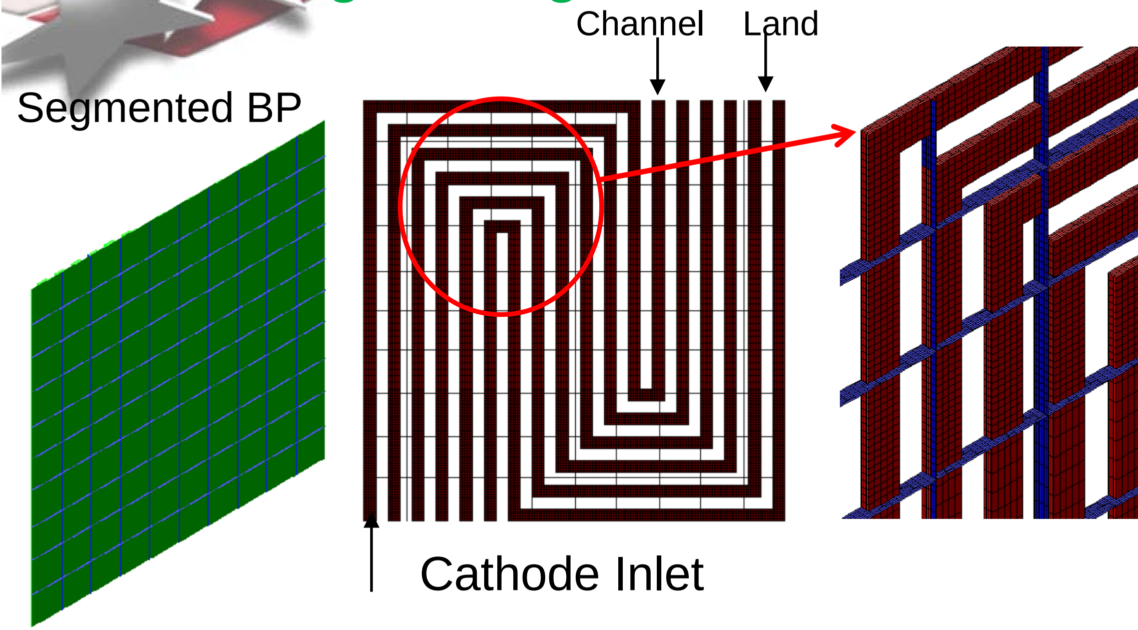
Parameters	Values
Cell size	50 [cm^2]
Channel height	1 [mm]
Temperature, T	60 [°C]
Flow velocity, u	10 [m/s]
GDL contact angle, θ_s	120 [°]
Net-transport coefficient, β	0.3
Water vapor fraction, α [1]	0.56 at 80 °C 0.22 at 60 °C
Critical droplet size [2]	1 [mm]
GDL surface tension	0.072 [N/m]

$$N_w = \frac{i}{F}\left(\beta + \frac{1}{2}\right) - \frac{i}{2F}\alpha$$

$$\beta = 0.2191\, i^{-0.374}, \text{ where } i \text{ is in A/cm}^2 \quad [3]$$

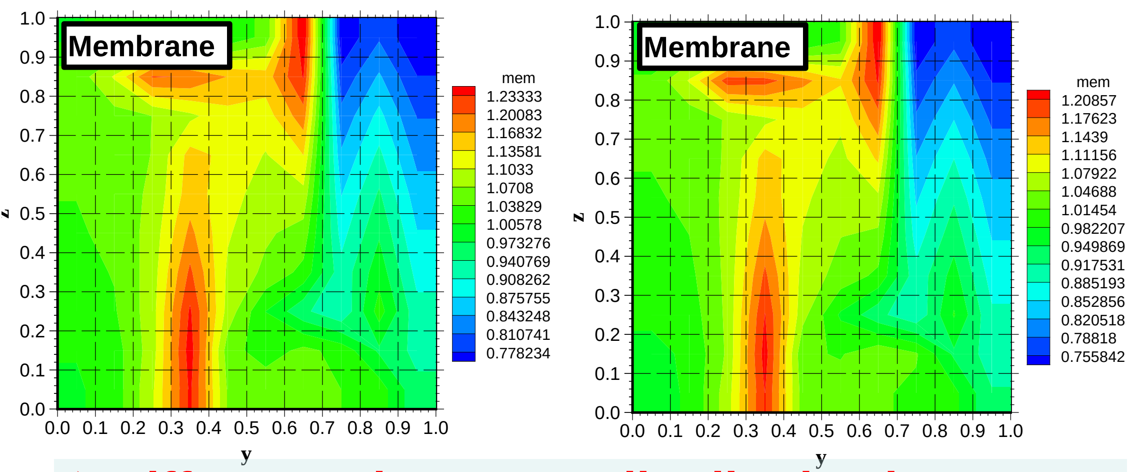
[1] A.Z. Weber, M.A. Hickner, *Electrochimica Acta* 53 (2008) 7668–7674.
[2] K. S. Chen, *Proc. Int. Conf. on Fuel Cell Sci., Eng. & Tech.*, June 16–18, 2008, Denver, Colorado.
[3] Q. Yan, H. Toghiani, J. Wu, *Journal of Power Sources* 158 (2006) 316–325.

Technical accomplishment: Computed effect of cell segmenting on current distribution measurement



Current density distribution

Non-segmented | **Segmented (10x10)**



➢ **Difference in current distribution between non-segmented and segmented cells < 4%!**

Questions:

1. **Are we measuring the right thing?**
2. **What is the best practice of cell segmenting?**

- **Bipolar plate segmentation has negligible effect on current distribution in the membrane when done properly.**
- **To reduce discrepancy, some guidelines need to be followed:**

  1) Segmentation along the flow direction

  2) Large errors seen mostly in U-turn regions where a segment contains mixed and irregular types of regions with flow channels and lands.

  3) Cutting through channels or land non-symmetrically in segmentation yields unacceptable errors in current distribution measurements.

Experimental apparatus and setup at LANL for polarization & current distribution measurements

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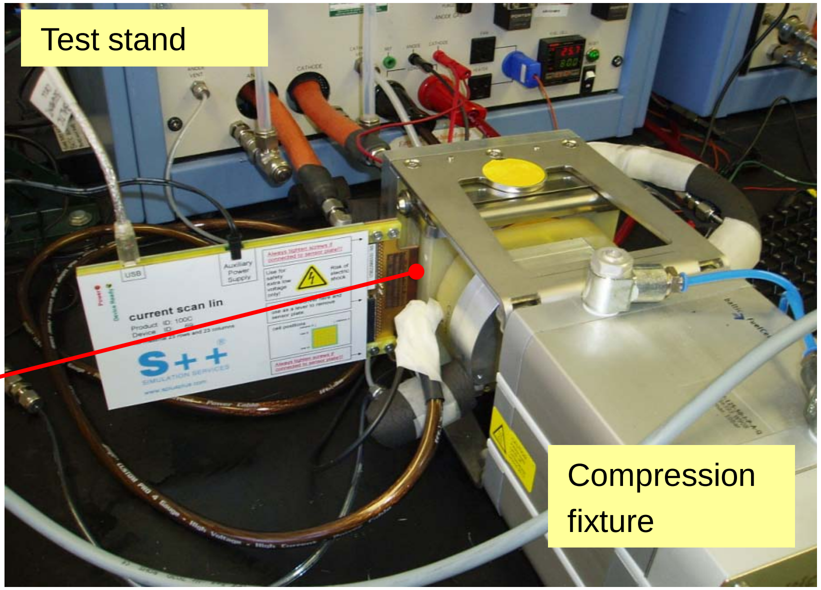
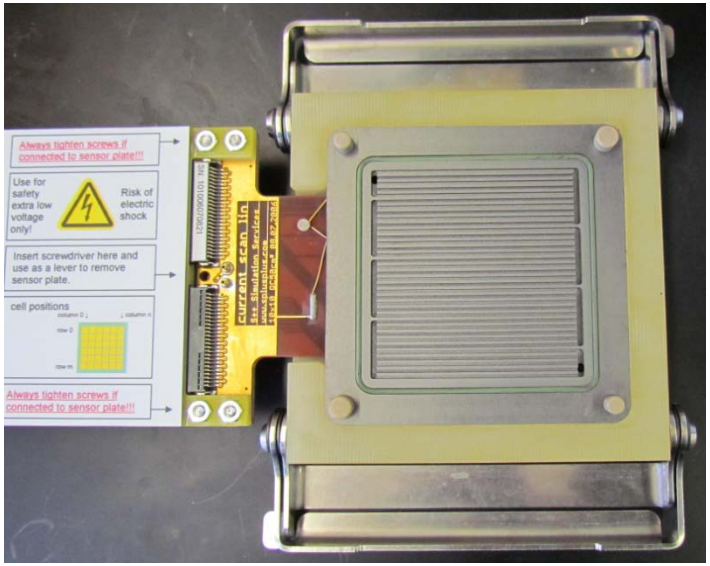
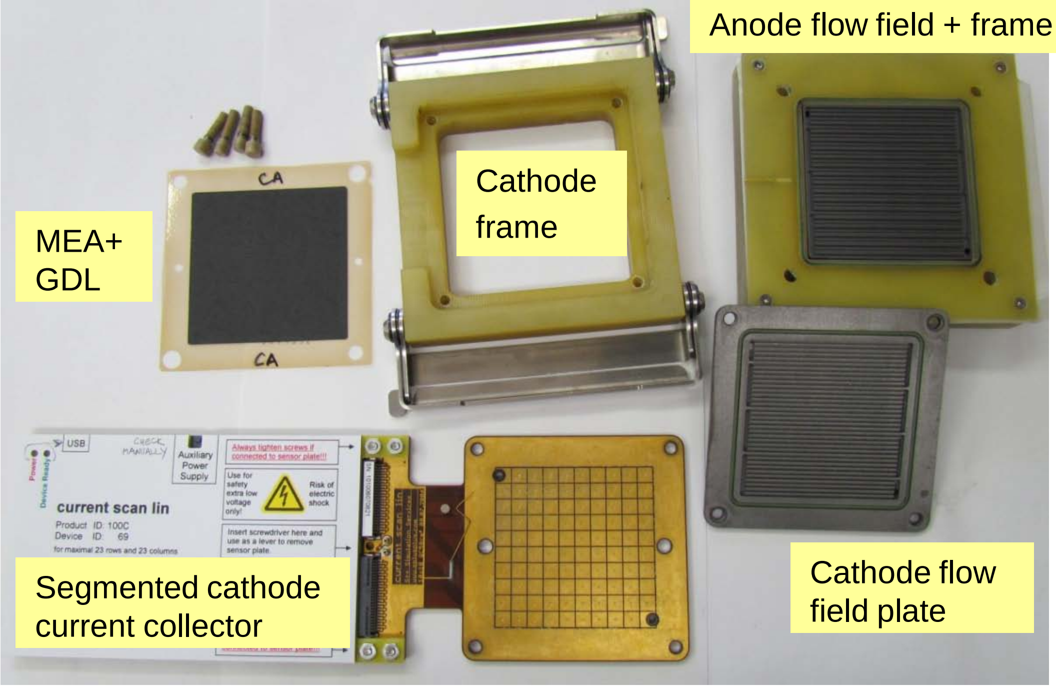
Fuel Cell Assembly 50 cm²
- Current and T Distribution (10 x 10 segments)
- Varying Compression

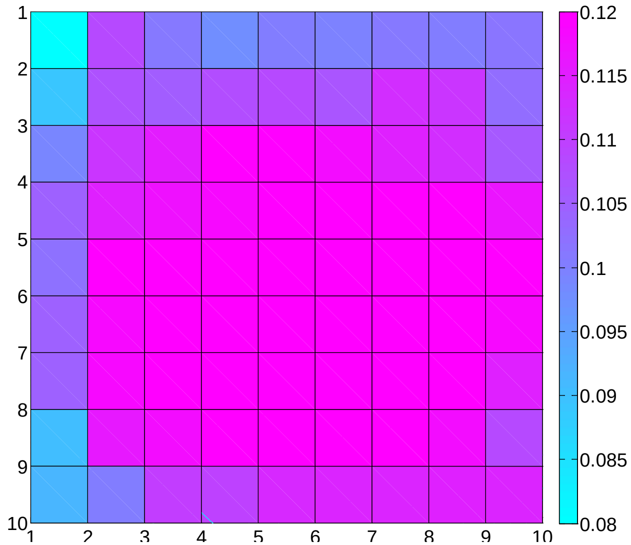






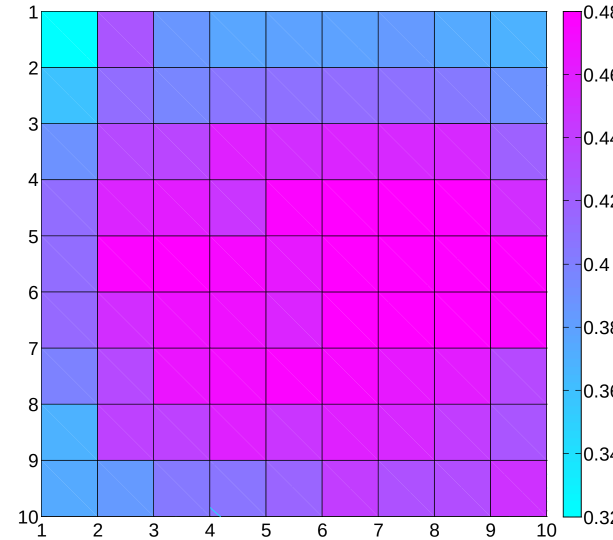
Technical accomplishment: Current distribution maps obtained using LANL's 10x10 segmented cell

Cell Area = 50 cm^2, Flow Field = 5-pass serpentine with manifolds, Segmented Current Collector = 10 x10 segments
MEA (catalyst coated membrane) = A510.2/M710.18/C510.4 (by W. L. Gore), GDL = SGL24BC (by SGL Carbon)
GDL – 200μm, MPL – 50μm, cathode CL – 20μm, anode CL – 10μm, membrane – 18μm.



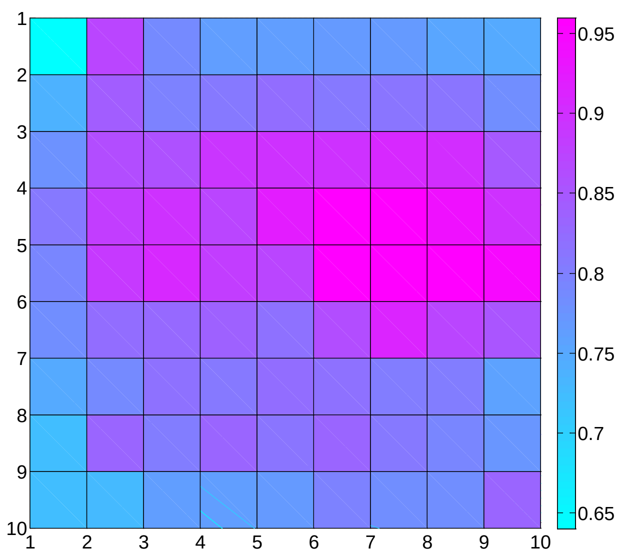
A/cm^2

I = 0.1 A/cm^2



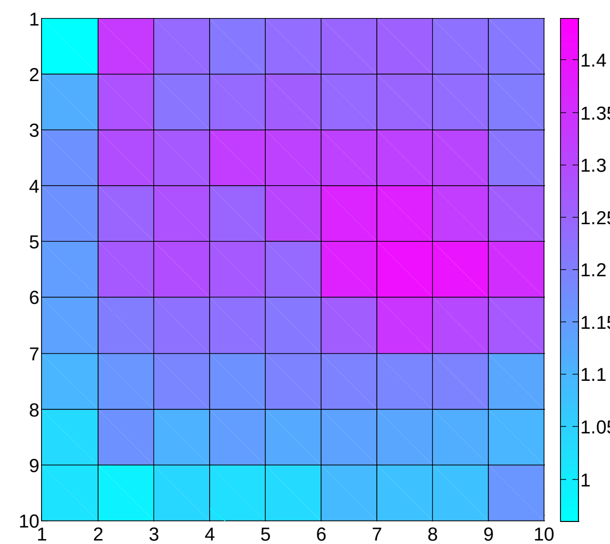
A/cm^2

I = 0.4 A/cm^2



A/cm^2

I = 0.8 A/cm^2



A/cm^2

I = 1.2 A/cm^2

Technical accomplishment: Simultaneous current & temperature distribution measurements

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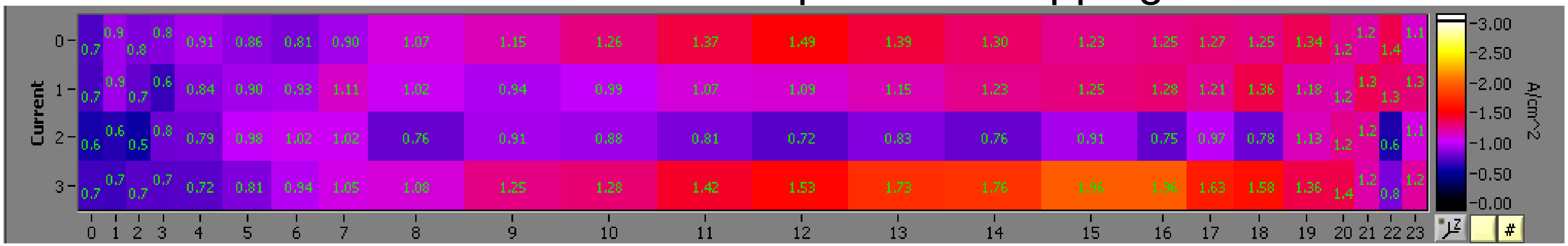
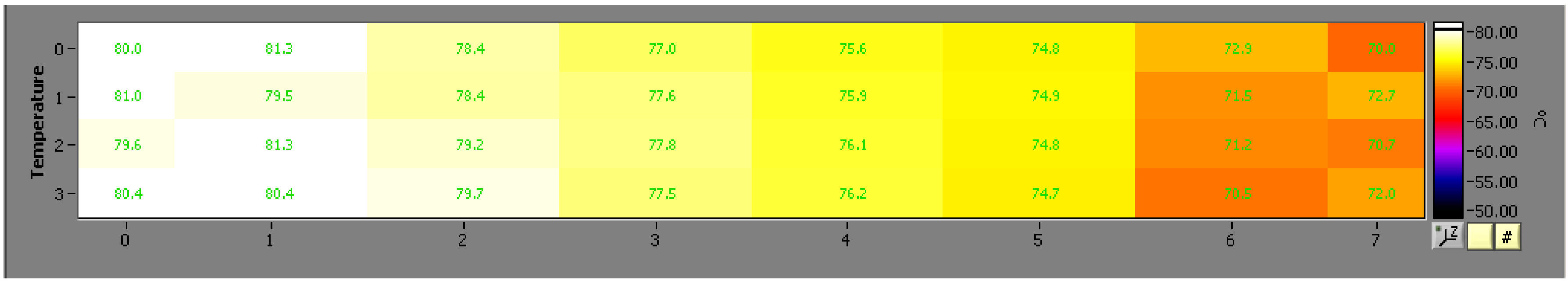
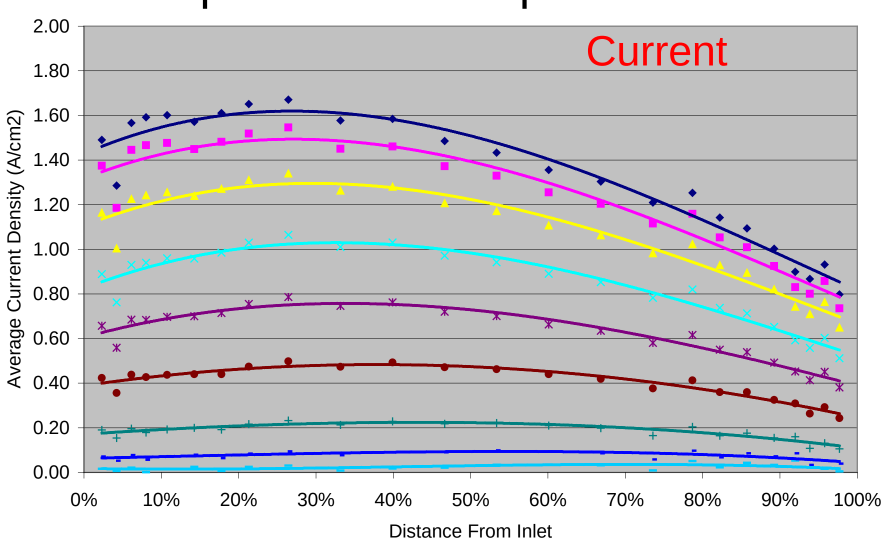
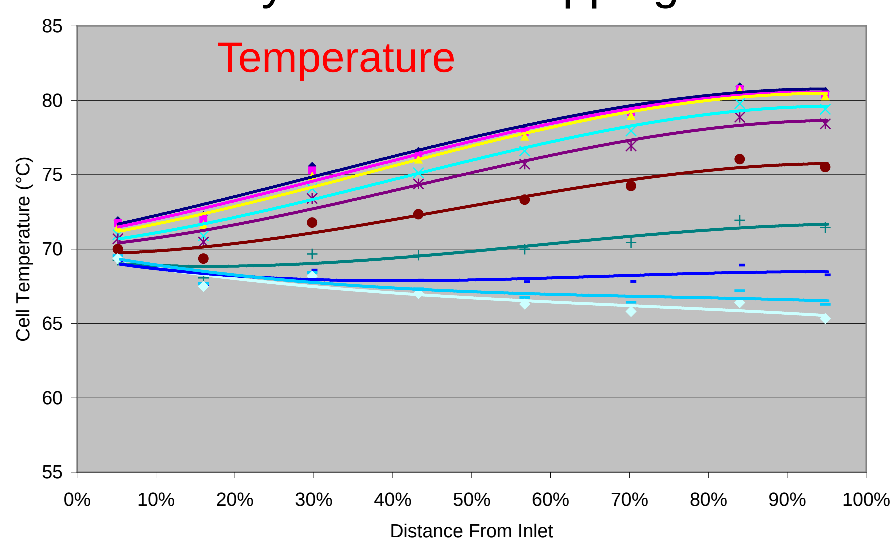
Ballard's current and temperature mapping tool





Sample current/temperature distribution obtained by Ballard's mapping tool





Technical accomplishment: Polarization curves with upper and lower bounds (Ballard)

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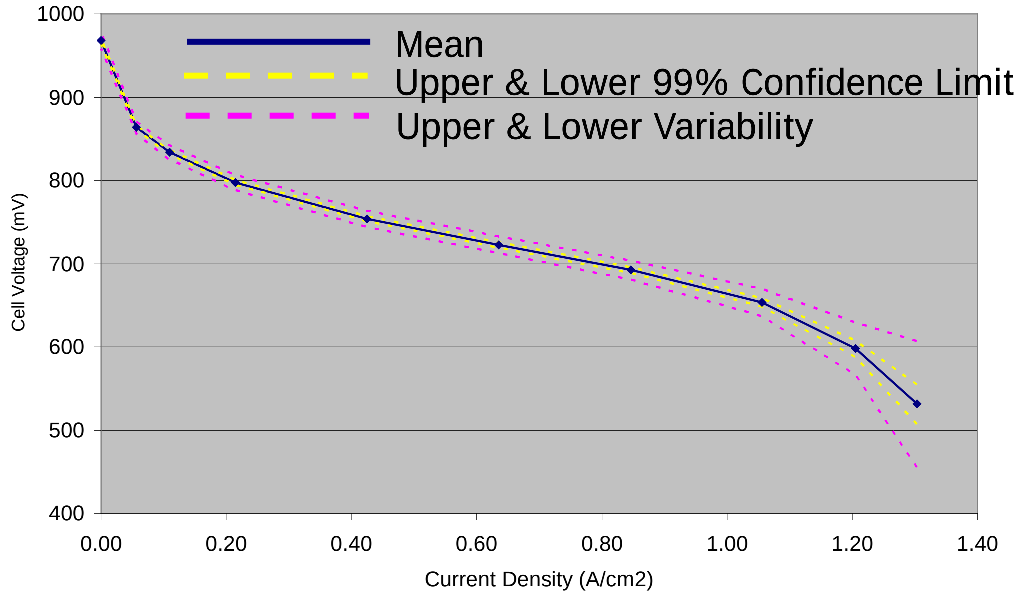
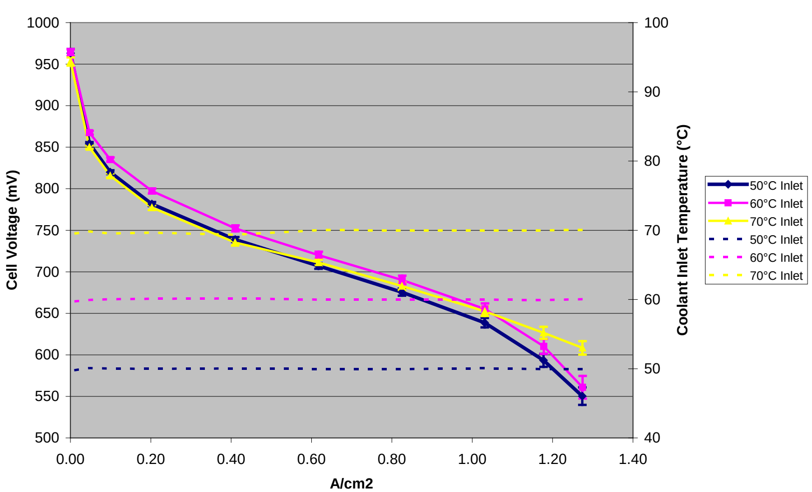
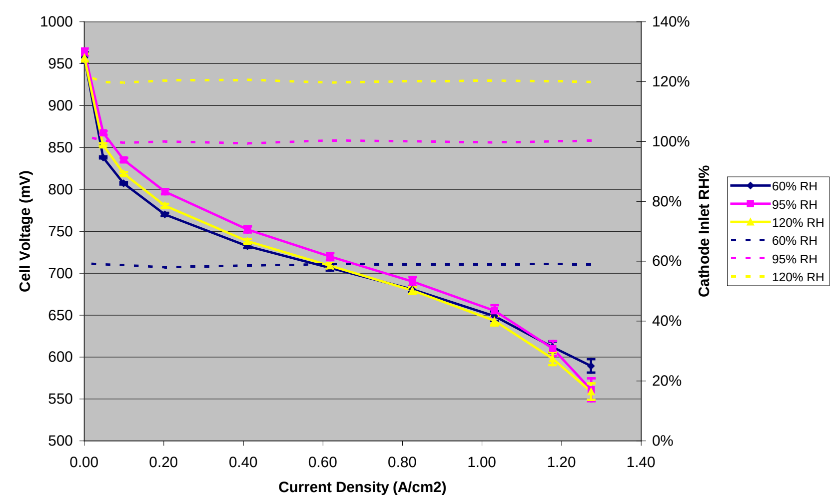


Sample polarization curve with upper and lower bounds

Temperature sensitivity



RH sensitivity



Validation Procedure

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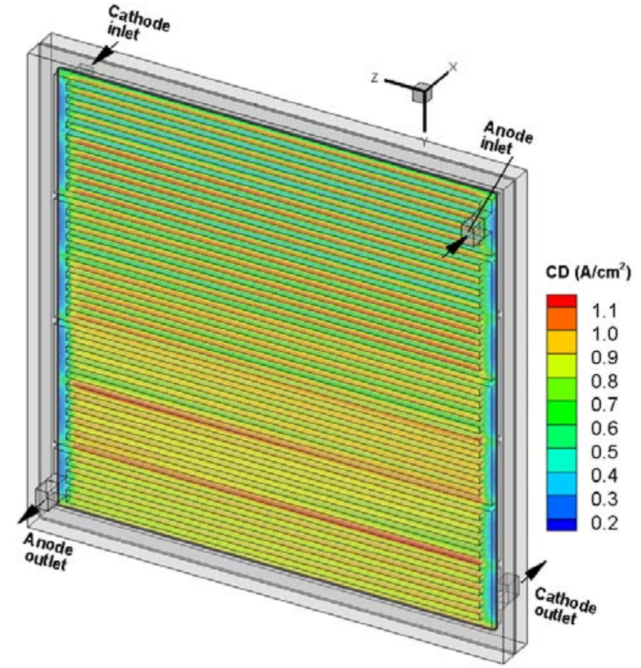
- Data collection milestone (led by LANL)
  - 80C, 100-75-50-25RH, 0.1-0.4-0.8-1.0-1.2 A/cm2
  - 60C, 100-50RH, 0.1-0.4-0.8-1.0-1.2 A/cm2
  - uncertainty quantification (error bars on the data)
- Mesh and model generation based on LANL experimental setup
  - Generate sequence of meshes
- Verification:
  - Geometric and model input parameters
  - Mesh convergence
- Initial calculations (no parameter adjustments)
- Sensitivity analysis (determine key model parameters)
- Calibration using subset of data – 80°C/50 RH/0.8 A/cm^2
- Validation against remaining LANL data
- Uncertainty quantification (error bars on the simulations)
- Summer 2011: testing and validation against Ballard data

Predicted membrane current distribution



<u>Operating conditions:</u>

Stoich(a/c): 1.2/2

Pressure(a/c): 1.95 atm

<u>Materials/geometry:</u>

Gore MEA (18 μm mem.)

Pt (a/c): 0.2/0.4 mg/cm^2

Cell area: 50 cm^2

Technical accomplishment: Model Validation: I-V Curves

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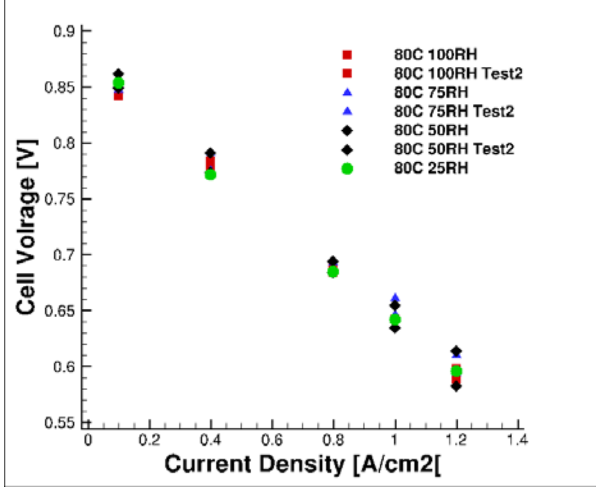
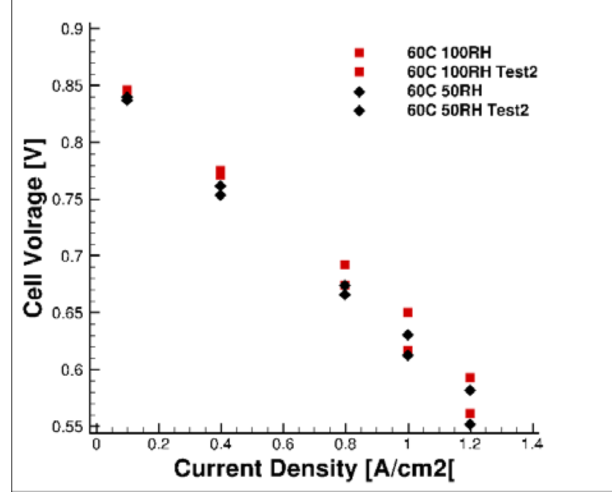
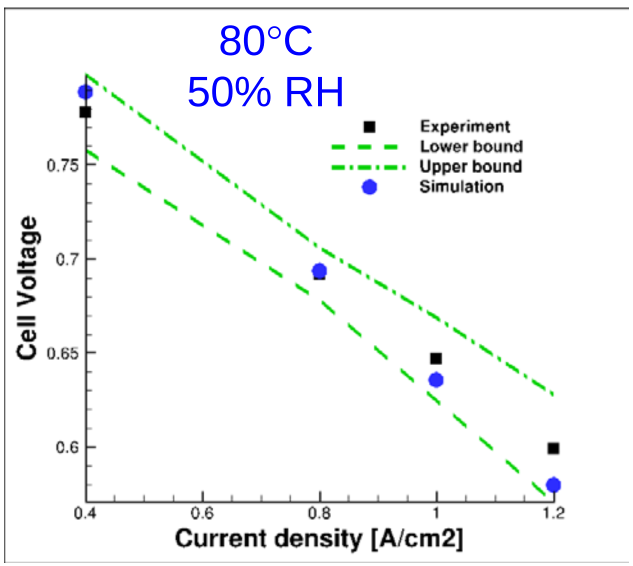
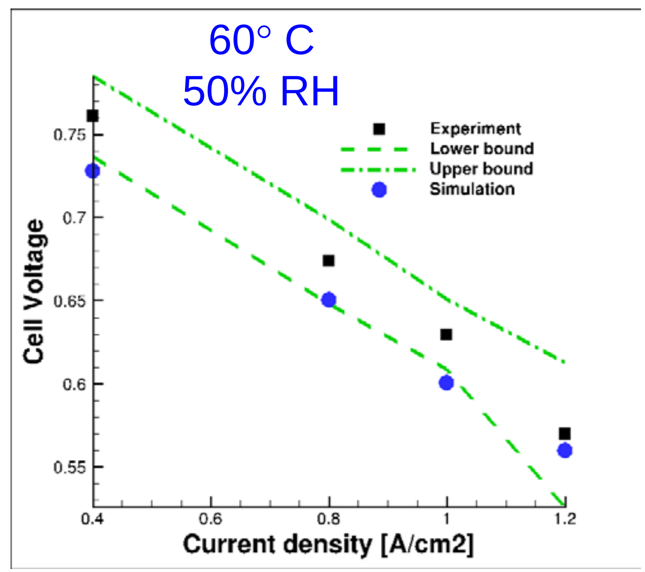
Experimental data from LANL at 80°C and 60°C (note variability)









- **Model calibration at 80°C and prediction at 60°C are within uncertainty of the experimental data!**

Technical accomplishment: Validation: Current Distribution

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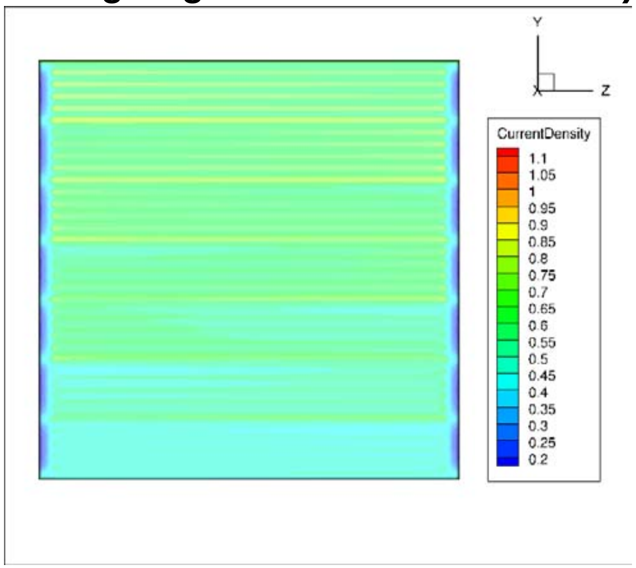
Detailed model prediction of current density (0.5mm grid gives 140x140 resolution)



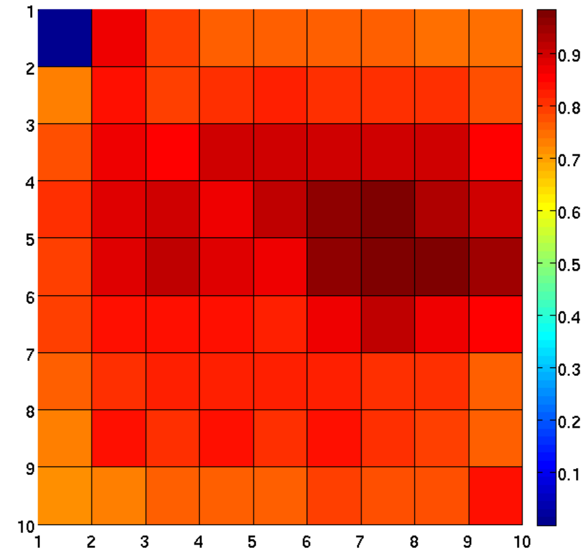
Operating Conditions: (Case 1)

80° C

50% RH

0.8 A/cm^2

Current density map of segmented cell data obtained by LANL (10x10 cell)



Model prediction

Inlet	0.74	0.75	0.75	0.75	0.76	0.76	0.77	0.78	0.70
0.62	0.73	0.73	0.73	0.73	0.73	0.73	0.74	0.74	0.66
0.67	0.78	0.77	0.76	0.76	0.75	0.75	0.74	0.74	0.64
0.65	0.78	0.79	0.80	0.81	0.82	0.82	0.83	0.84	0.72
0.70	0.83	0.83	0.83	0.83	0.83	0.83	0.83	0.83	0.73
0.74	0.87	0.87	0.86	0.86	0.86	0.85	0.85	0.85	0.72
0.68	0.84	0.85	0.86	0.87	0.87	0.88	0.89	0.90	0.76
0.76	0.92	0.92	0.91	0.91	0.90	0.90	0.89	0.89	0.74
0.74	0.90	0.90	0.89	0.89	0.89	0.89	0.88	0.88	0.74
0.61	0.74	0.74	0.75	0.75	0.76	0.76	0.77	0.77	Outlet

Experimental data

Inlet	0.87	0.79	0.76	0.76	0.77	0.77	0.75	0.75	0.75
0.73	0.84	0.79	0.80	0.82	0.81	0.81	0.81	0.78	0.80
0.77	0.86	0.86	0.89	0.90	0.89	0.91	0.90	0.85	0.83
0.81	0.88	0.90	0.87	0.92	0.97	0.98	0.94	0.90	0.89
0.80	0.89	0.91	0.88	0.87	0.97	0.98	0.98	0.95	0.92
0.79	0.83	0.84	0.85	0.82	0.87	0.91	0.88	0.85	0.89
0.75	0.80	0.83	0.82	0.83	0.83	0.81	0.81	0.76	0.82
0.73	0.83	0.81	0.83	0.82	0.83	0.81	0.79	0.77	0.82
0.72	0.73	0.76	0.76	0.77	0.80	0.78	0.78	0.83	0.76
0.68	0.70	0.60	0.53	0.71	0.68	0.69	0.72	0.59	Outlet

- **Currently we are within 15% on 90/100 cells with RMS error <12% for all cells. We are continuing efforts to improve model prediction to be within 10-15% on nearly all cells.**

Technical accomplishment:

More Validation: Current Distribution

Sandia National Laboratories

Model prediction

0.31	0.36	0.37	0.37	0.37	0.37	0.38	0.38	0.39	0.34
0.33	0.39	0.39	0.39	0.39	0.39	0.39	0.39	0.39	0.34
0.35	0.41	0.41	0.41	0.40	0.40	0.40	0.39	0.39	0.33
0.33	0.40	0.41	0.41	0.42	0.42	0.42	0.42	0.43	0.36
0.36	0.43	0.43	0.43	0.43	0.43	0.43	0.43	0.42	0.36
0.36	0.44	0.44	0.44	0.43	0.43	0.43	0.43	0.42	0.36
0.34	0.42	0.42	0.43	0.43	0.43	0.44	0.44	0.44	0.37
0.36	0.43	0.43	0.43	0.43	0.43	0.42	0.42	0.42	0.35
0.35	0.42	0.42	0.42	0.42	0.42	0.42	0.41	0.41	0.35
0.31	0.37	0.37	0.38	0.38	0.39	0.39	0.39	0.39	0.34

Experimental data

0.00	0.43	0.39	0.38	0.38	0.38	0.38	0.37	0.37	0.37
0.36	0.41	0.40	0.41	0.41	0.41	0.41	0.40	0.39	0.39
0.39	0.43	0.44	0.46	0.45	0.46	0.45	0.45	0.42	0.42
0.41	0.46	0.46	0.45	0.48	0.50	0.50	0.48	0.45	0.45
0.41	0.48	0.49	0.47	0.46	0.51	0.53	0.53	0.49	0.48
0.41	0.45	0.47	0.47	0.46	0.49	0.51	0.49	0.48	0.49
0.40	0.43	0.47	0.47	0.48	0.47	0.46	0.46	0.43	0.45
0.37	0.44	0.44	0.46	0.45	0.46	0.45	0.44	0.43	0.44
0.37	0.38	0.40	0.41	0.42	0.44	0.43	0.43	0.45	0.40
0.35	0.36	0.31	0.28	0.38	0.36	0.37	0.38	0.31	0.00

Operating Conditions:(Case 2)

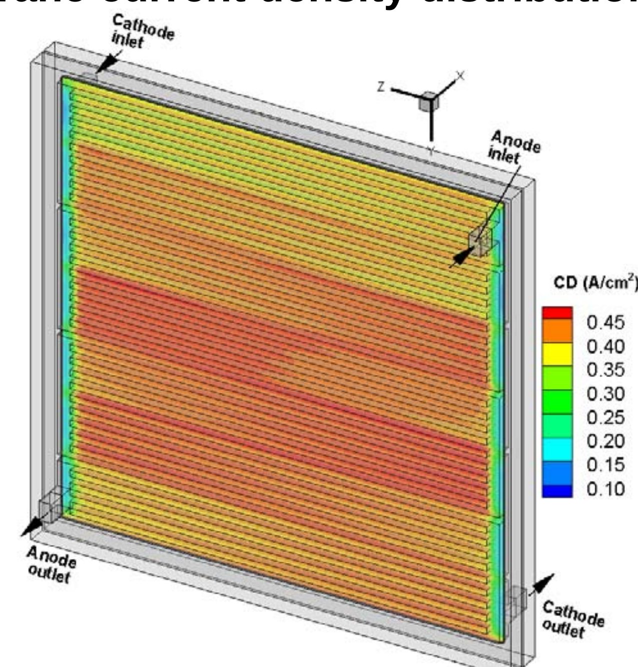
80°C, 50% RH, 0.4 A/cm^2

Relative difference between experimental data and model prediction

0.0%	15.3%	5.4%	2.1%	1.8%	1.4%	1.5%	-1.7%	-4.5%	8.8%
7.9%	4.7%	0.9%	4.0%	4.2%	4.7%	4.6%	3.3%	-0.4%	13.4%
11.4%	5.3%	6.7%	11.7%	11.0%	12.1%	12.2%	13.0%	6.4%	19.7%
19.7%	11.6%	11.6%	7.9%	13.0%	16.6%	16.4%	11.5%	5.4%	19.3%
12.7%	9.4%	11.2%	9.1%	7.1%	15.2%	18.8%	19.4%	14.3%	24.0%
12.1%	2.9%	6.8%	7.2%	4.8%	11.7%	16.0%	13.3%	10.9%	26.0%
15.7%	4.2%	9.4%	9.6%	9.3%	8.1%	5.5%	4.5%	-1.8%	17.5%
3.0%	1.1%	1.2%	5.9%	3.8%	7.0%	6.5%	4.9%	2.3%	19.7%
7.3%	-8.9%	-4.0%	-3.1%	-1.1%	4.9%	2.6%	3.7%	8.6%	12.7%
11.2%	-1.8%	-19.6%	-35.0%	-0.7%	-5.5%	-4.5%	-1.6%	-27.6%	0.0%

- **Agreement between computed and measured current density distribution is good with RMS error < 11.3%!**

Predicted membrane current density distribution



PEMFC Model Demo: Overview of code and files

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- The code is based on FLUENT with extensive user-defined functions (UDF) to provide additional capability.
- Prerequisites for the code are
  - the *.cas file ("Sample.cas")
  - the UDF library ("libudf")
  - an installation of FLUENT and C compiler
- Contents of the Sample.cas file
  - The computational mesh (including boundary/volume/interface zones)
  - Material and boundary condition specifications
  - Solver parameters

The user edits the main header file ("defineparam.h")

Setting input parameters

emacs@wsblade007.sandia.gov <10>

File Edit Options Buffers Tools C Help

```
/* Electrochemical Properties */
double ajo_a_ref =1.0e9;          /* Anode reference ex current density
double ajo_c_ref =1.0e4;      /* Cathode reference ex current density
double alptt_a =2.;           /* Total Anode Transfer Coefficient
double alptt_c =1.;           /* Total Cathode Transfer Coefficient
double Ch2_ref =40.;          /* Reference hydrogen concentration
double Co2_ref =40.;          /* Reference oxygen concentration
double Fr =96487.0;           /* Faraday's constant [96487 C/mol]
double cor_aj0 =8000.;       /* coefficient accounting for temperature effect on ajo_*_r

/* Physical Properties */
double EW =1.1;               /* kg/mol
double rhodry =1.98e3;        /* kg/m^3
double Runiv =8.314;         /* Universal gas constant [8.314 J/molK]

/* Operational Parameters */
double iavg_ref =1.3e+4;          /* Ref av current density for st. cof. defn. [A/m^2
double stoich_a =2.0;         /* Anode Stoichiometric Coefficient at 1 A/cm^2
double stoich_c =2.0;        /* Cathode Stoichiometric Coefficient at 1 A/cm^2
double pr_a =2.0;             /* Anode Inlet Pressure [atm]
double pr_c =2.0;             /* Cathode Inlet Pressure [atm]
double p_ref =2.0;            /* Reference Pressure [atm]
double T_gas_in_a  =353.15;       /* Gas Temperature [K] at anode inlet
double T_gas_in_c  =353.15;       /* Gas Temperature [K] at cathode inlet
double T_a =348.2;                /* Anode Water Saturation Temperature [K]
double T_c =348.2;                /* Cathode Water Saturation Temperature [K]
double T_cell =353.15;       /* Cell Temperature [K]
double V_c =0.6;                  /* Cell Voltage [V]   !Input!
double V_oc_80 =1.1749;          /* Open Circuit Voltage [V] at 353.15 K

/* Dry Hydrogen and Oxygen Percentage */
double h2percentage =1.0;        /* dry hydrogen percentage in anode inlet
double o2percentage =0.21;        /* dry oxygen percentage in cathode inlet

/* Molecular weight */
double mw_h2 =2.0;
double mw_o2 =32.0;
double mw_h2o =18.0;
double mw_n2 =28.0;

/* Membrane Water Diffusion Coefficient */
int i_mwd =4;                                  /* 1-- Motupally,2 -- half Springer,3
inger */
double c_spr =0.7;                             /* only meaningful when i_mwd=4 */
double D_hp_0 =1.5e-9;                         /* minimum diffusivity by hydrolic per

/* Membrane proton conductivity */
int F_memcond =1;                              /* 1 -- Springer 1990, 2 -- Sone 1996
double lambda_0 =1.0;

/* Parameters for M2 Model */
--(DOS)--  defineparam.h      (C Abbrev)--L31--Top--------------------------------
```

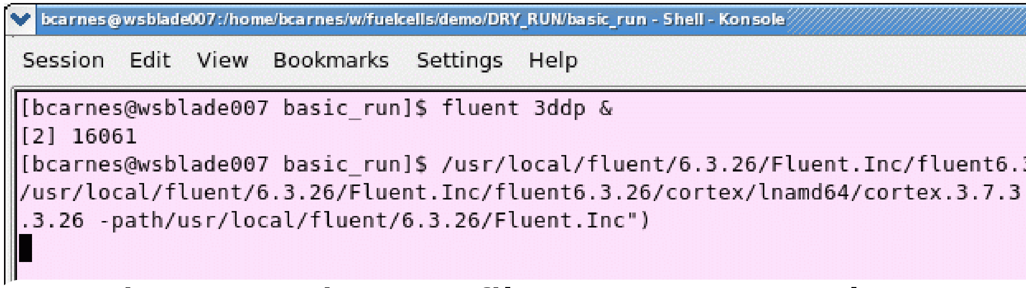
bcarnes@wsblade007:/home/bcarnes/w/fuelcells/demo/DRY

Session Edit View Bookmarks Settings

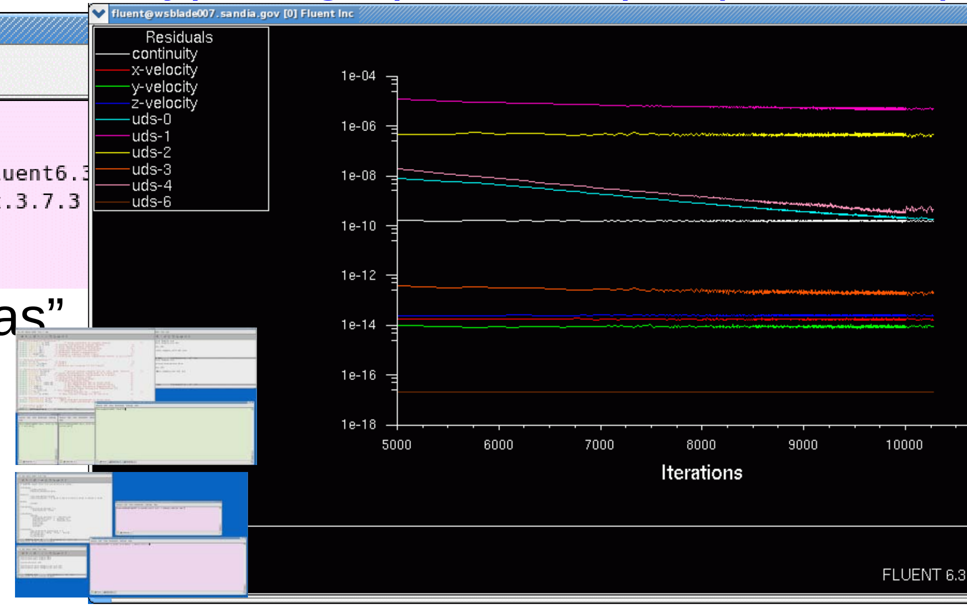
```
[bcarnes@wsblade007 basic_run]$ ls
clean.sh  libudf  output  Sample.cas
[bcarnes@wsblade007 basic_run]$ cd lib
[bcarnes@wsblade007 libudf]$ ls
lnamd64  Makefile  src
[bcarnes@wsblade007 libudf]$ cd src/
[bcarnes@wsblade007 src]$ ls
defineparam.h  ececpem_lib.h  ececpem_v1.0.c  ID_subregion.h  makefile
[bcarnes@wsblade007 src]$
```

Example: Basic run

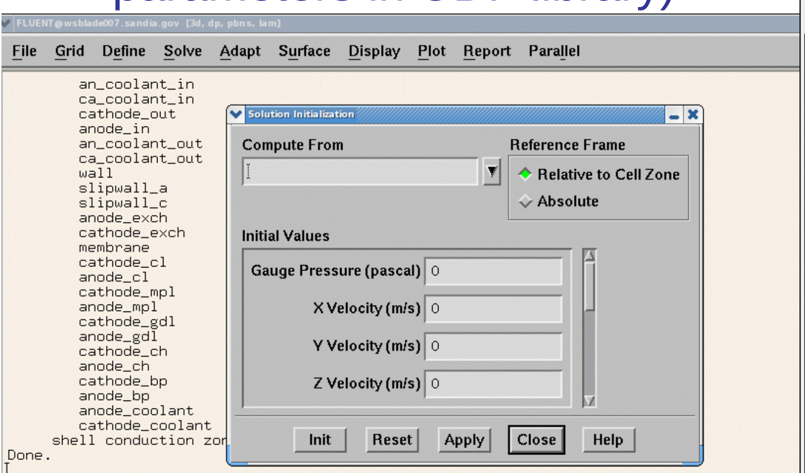
- We normally launch the code in a Linux environment
- To launch the GUI version in serial



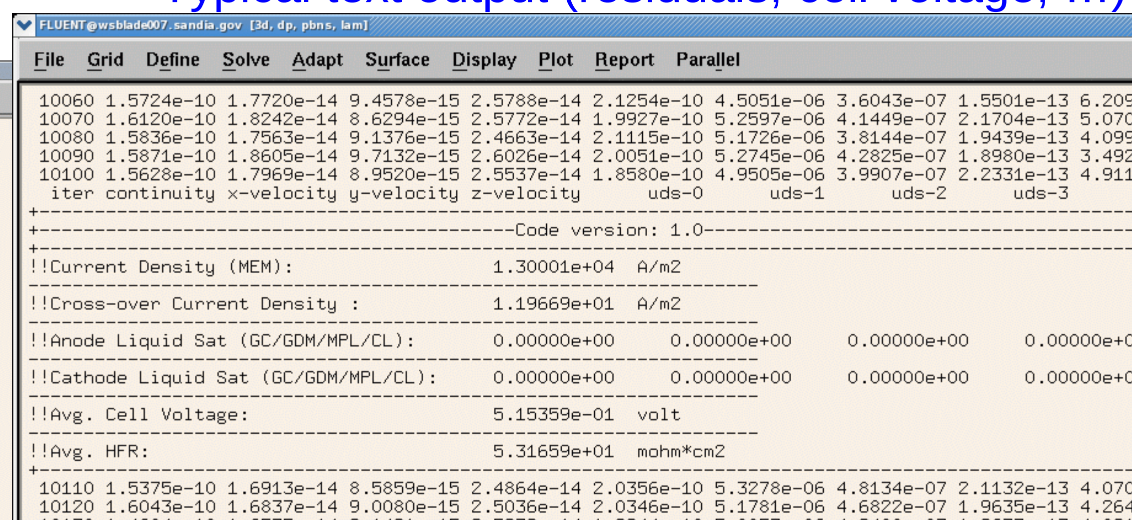
Typical graphical output (residuals)



- Then read case file, e.g., “Sample.cas”
  Initialization
  Using previously computed solutions (useful for polarization curves or parameter studies)
  From scratch (based on current parameters in UDF library)



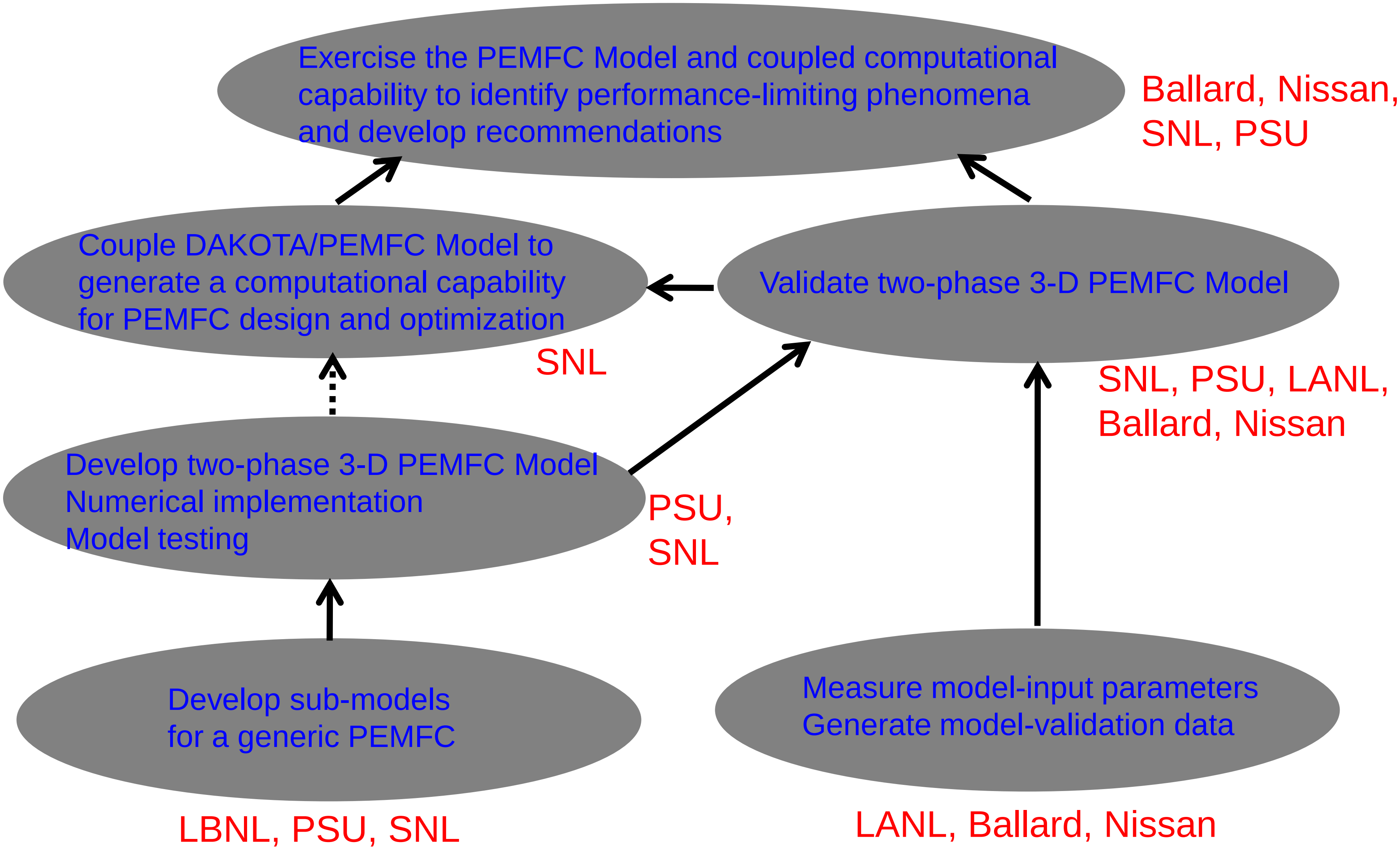
Typical text output (residuals, cell voltage, …)



Collaborations:

How team partners work together to achieve project objective?

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



Future Work

Remaining FY11:

1. Complete development and testing of the 3-D, fully two-phase, single-cell model

   Milestone M3: Develop a 3-D, *fully two-phase*, single-cell model and demonstrate model utility in case studies with acceptable numerical convergence measured by absolute residuals of 10^{-5} or less and mass/charge balance error of *2%* or less. Due: 6/30/2011

2. Complete model validation in the single-phase and partially two-phase regimes using LANL data from segmented cell experiments.

3. Perform model validation in the single-phase and partially two-phase regimes using test data from Ballard (polarization, current/temperature maps, etc.).

   Milestone M5: Perform validation of the 3-D, partially two-phase, single-cell model by comparing computed and measured polarization curves, and current distributions with reasonable agreement (errors fall into the *99%* confidence interval or within +/-*15%*). Due: 9/30/2011

FY12:

4. Complete sub-model and algorithm development, and numerical implementation.
5. Develop a 3-D, two-phase, short stack model.
6. Obtain water profiles in the through-plane using neutron radiography setup at NIST.
7. Perform model validation in the fully two-phase regimes using neutron imaging data obtained by LANL at NIST, and test data from Nissan and Ballard.

FY13: Exercise model to identify performance-limiting phenomena and develop recommendations so as to address technical barriers and support DOE objectives.

Summary of Technical Accomplishments

- Year 2 experimental milestone M4 ("Measure *10*x*10* current distribution performance data for model validation for 4 different operating conditions (RH = *25%*, *50%*, *75%* and *100%*)") was successfully completed.
- A 3-D, fully two-phase, single-cell model was developed and demonstrated in parametric studies; the Year 2 modeling milestone M3 ("Develop a 3-D, fully two-phase, single-cell model") is near completion.
- Significant progress has been made in model validation using polarization and current distribution data obtained by LANL using a *10*x*10* segmented cell. Year 2 model-validation milestone M5 is on track.
- Other accomplishments include:
  - Demonstrate the fully two-phase model by simulating a PEMFC with a Chevron flowfield.
  - A nonisothermal pore network model was developed and demonstrated.
  - 3-D CFD simulation was performed to verify the analytical model for droplet detachment.
  - Simplified calculations were performed to estimate water flux at GDL/channel interface.
  - Effect of cell segmenting was investigated and segmentation guidelines were developed.
  - Current/temperature maps and polarization curves with upper/lower bounds were obtained.
- 3 journal publication, 3 proc. papers and 6 conference presentations were generated.

Technical Back-Up Slides

An approximate but robust approach for accounting for MPL effect

Parameters: ε_{GDL} = 0.6, K_{GDL} = 10^{-12} m^2, $\theta_{c,GDL}$ = 92^o, ε_{MPL} = 0.4, K_{MPL} = 10^{-13} m^2, $\theta_{c,MPL}$ = 150^o, H_{GDL} + H_{MPL} = 200 μm

Motivation: to eliminate the need for numerically treating the MPL/GDL interface with steep saturation jump.

Approach: treat MPL/GDL as a composite component with effective properties (ε, K, θ_c).

From pore volume being additive:

$$\varepsilon_{MPL-GDL} = \varepsilon_{MPL}\frac{H_{MPL}}{H_{MPL}+H_{GDL}} + \varepsilon_{GDL}\frac{H_{GDL}}{H_{MPL}+H_{GDL}}$$

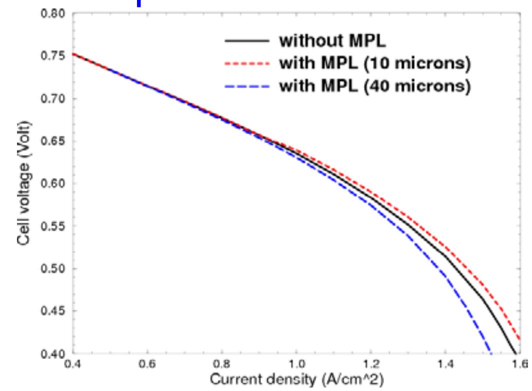
From flow resistance being additive:

$$K_{MPL-GDL} = \frac{1}{\frac{1}{K_{MPL}}\frac{H_{MPL}}{H_{MPL}+H_{GDL}} + \frac{1}{K_{GDL}}\frac{H_{GDL}}{H_{MPL}+H_{GDL}}}$$

From capillary-pressure being additive:

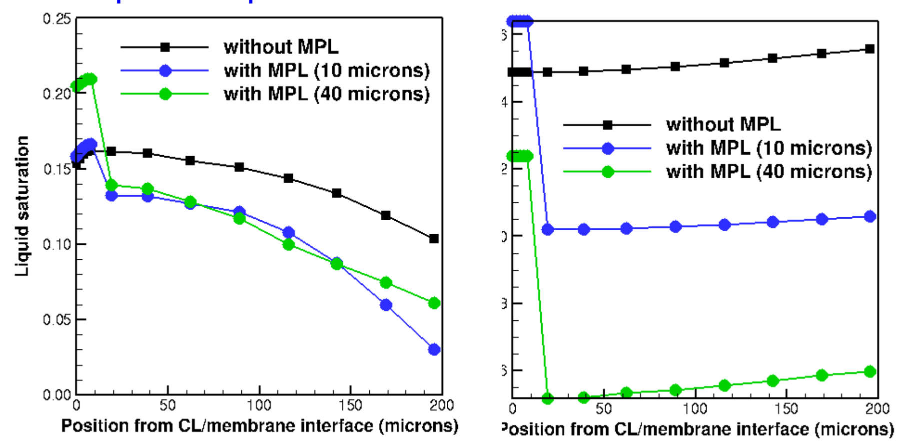
$$\cos\theta_{c,MPL-GDL} = \cos\theta_{c,MPL}\left(\frac{\varepsilon_{MPL}}{\varepsilon_{MPL-GDL}}\frac{K_{MPL-GDL}}{K_{MPL}}\right)^{1/2}\frac{H_{MPL}}{H_{MPL}+H_{GDL}} + \cos\theta_{c,GDL}\left(\frac{\varepsilon_{GDL}}{\varepsilon_{MPL-GDL}}\frac{K_{MPL-GDL}}{K_{GDL}}\right)^{1/2}\frac{H_{GDL}}{H_{MPL}+H_{GDL}}$$

Computed effect of MPL on cell performance



- MPL improves cell performance slightly when it is thin but hurts performance when sufficiently thick!

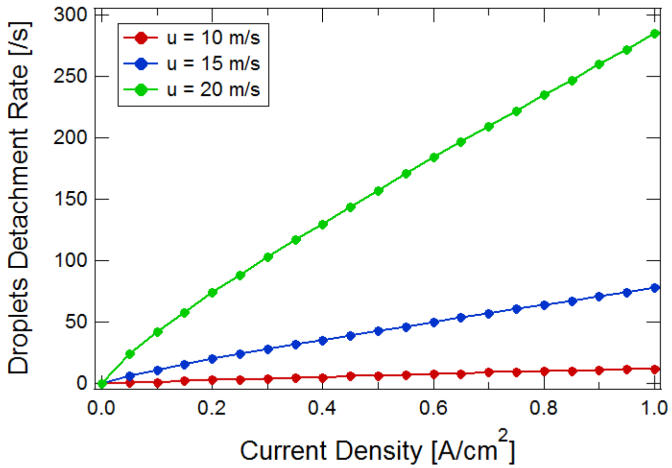
Computed liquid saturation across CL and MPL/GDL



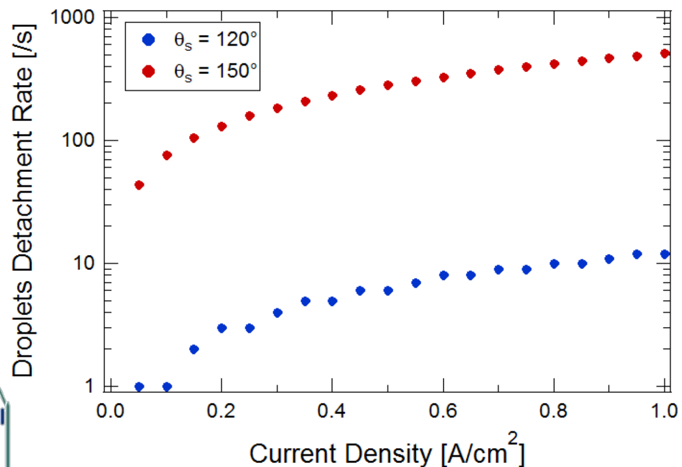
- Incorporating hydrophobic MPL reduces liquid saturation in MPL/GDL, particularly under the land!

Back-of-Envelope Calculation: Droplets

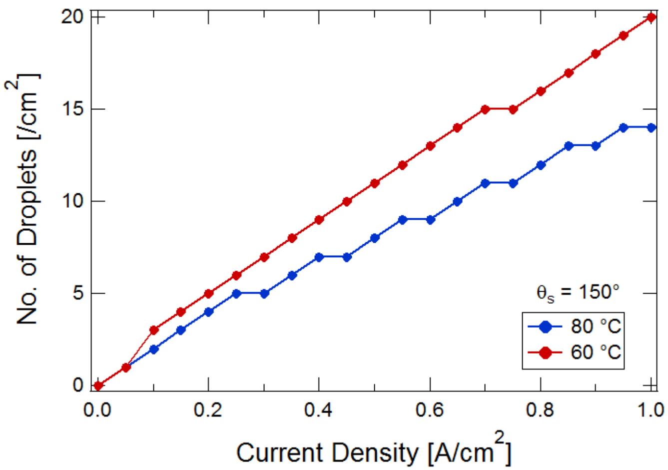
- Droplet detachment
  - Gas flow velocity



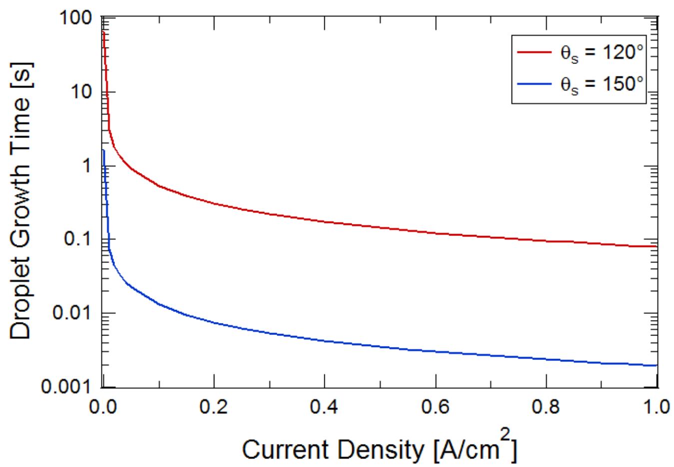
  - Surface static contact angle



- Droplets on surface
  - Number of droplets



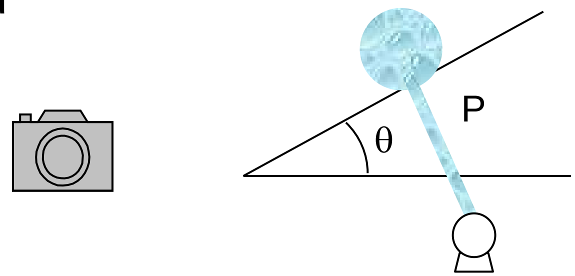
  - Growth of droplets



Droplet Imaging Experiment

Goal: Improve models and understand droplet governing physics

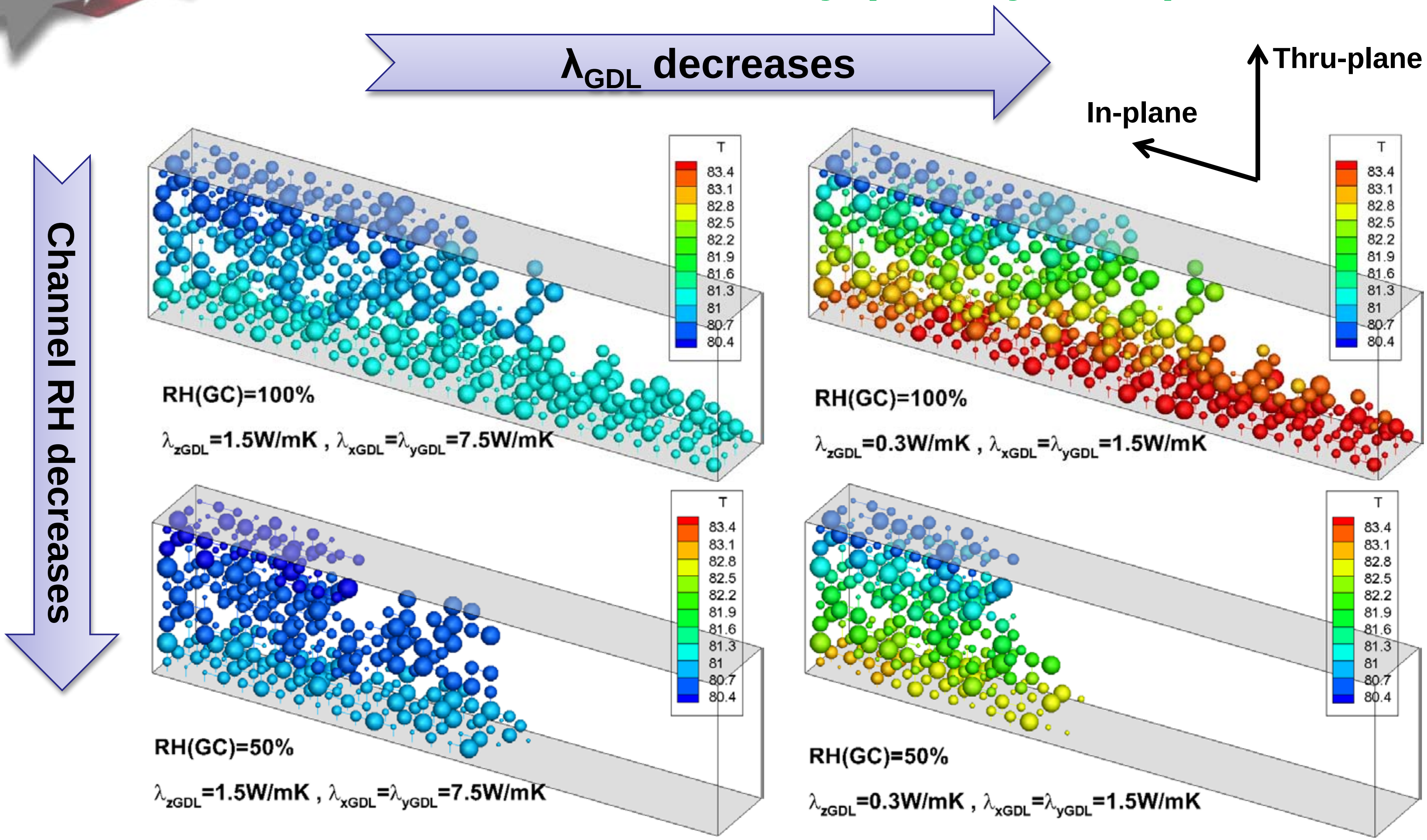
- Directly measure the adhesion force instead of depending on contact-angle measurements and hysteresis
  - Measure angle at which droplet begins to move and liquid pressure
- Measure real and ideal materials with liquid water injected



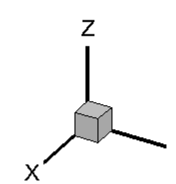
  - Understand the impact of pore size and injection rate of liquid supply
  - Look at both ideal and real GDLs (including multiple droplets)
    - Identify droplets growth in an unit area
- Vary materials, droplet sizes, injection flow rates and sizes, existence of channels and flow

Goniometer with Tilt Stage

Pore network modeling: Effect of channel RH and GDL thermal conductivity (steady state)



Lower thermal conductivity & channel RH result in less GDL flooding!



Sensitivity Analysis Using PEMFC/DAKOTA Coupled Model

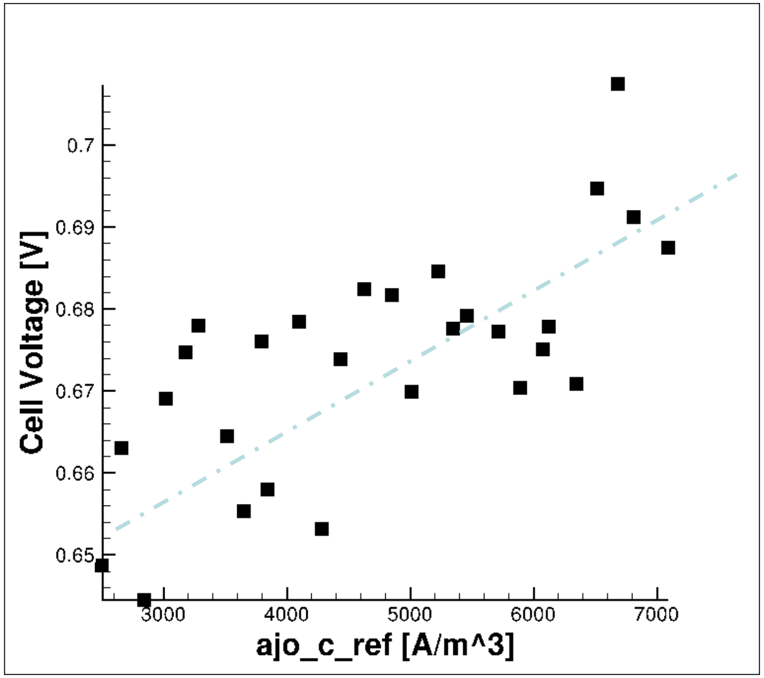
Efficient sensitivity analysis is enabled using the PEMFC/DAKOTA coupled model.

Here we varied 22 parameters to determine the ones with greatest impact on cell voltage.

Linear regression predicts effect of parameter on performance. Positive R value indicates positive correlation.

Cathode exchange current density was most important parameter, followed by anode CL porosity.

param	R	m	b
ajo_c_ref	0.71	7.06E-006	0.64
eps_cl_a	-0.57	-0.07	0.71
eps_mpl_c	0.2	0.02	0.66
eps_cl_c	0.16	0.02	0.66
k_p_bl_c	0.13	6.85E+009	0.67
eps_bl_a	-0.13	-0.02	0.68



Thanks to

U. S. DOE EERE Fuel Cell Technologies Program for financial support of this work

– Program Managers: Jason Marcinkoski
Donna Ho

Reviewer-Only Slides

Addressing reviewers' comments from 2010 AMR

- Comment: Collaborative efforts could be a little stronger. Partners seem academia heavy.

  Response: Model development involves one university (PSU) and two national labs (SNL and LBNL). Experimental and validation results come from one national lab and two industrial partners (Ballard and Nissan). We tend to believe that a strong academic presence is a good thing in that it provides a strong theoretical background which is important for such a modeling project. Lastly, the collaboration with industry will become more apparent later this year and in Years 3 and 4, when the model input data and performance data provided by Ballard and Nissan are utilized in model validation, and when Ballard and Nissan start to run the PEMFC model and the coupled DAKOTA/PEMFC model computational capability.

- Comment: This project obviously requires a lot of collaboration, since all of the team members must provide substantial input to generate the complex model of the sort envisioned here, especially if the model is also going to be validated (instead of just being used to "predict general trends"). It is also good that the project has an original equipment manufacturer (OEM) like Ford participating with no funding from DOE.

  Response: Nissan has replaced Ford in our project. We are fortunate to have Nissan's participation in this project "with no funding from DOE". We consider Nissan's involvement, and guidance/insights and parameter ranges, etc. provided by Nissan to be very important to the success of this project.

Addressing reviewers' comments from 2010 AMR (Continued)

- Comment: The proposed approach of continuing to the partial two-phase model with the validation of the current model seems to be sound. The continued incorporation of the DAKOTA approach to make the model predictive and allow for uncertainty is good. I think it is important to address the water flux as described in the future work.

  Response: Thanks for the positive comments. Yes, it is important to "address the water flux as described in the future work". Specifically, Adam Weber of LBNL is leading this effort to develop a submodel for properly accounting for water flux at the GDL/channel interface.

- Comment: The approach of modeling the behavior and trying to build in the uncertainty is an important step. The focus on generating good data for the model, under a range of conditions, as well as gathering fundamental data on the mass transport and the effect of materials properties, is a definite strength.

  Response: Thanks for the positive and encouraging comments.

- Comment: Validation of the modeling to date is weak.

  Response: We've made significant progress in model validation this year. Model validation will be continued in the remaining of this year and also in Years 3 and 4. It should be noted that model validation is being carried out using data obtained by LANL on their segmented cell. In the next stage of model validation, we plan to use cell design and data provided by original equipment manufacturer (OEM) Ballard.

Publications and Presentations

1. Y. Wang and K. S. Chen, "Through-plane water distribution in a polymer electrolyte fuel cell: comparison of numerical prediction with neutron radiography data", *J. Electrochem. Soc.* **157** (12) B1878−B1886 (2010).
2. Y. Ji, G. Luo,a nd C.-Y. Wang, "Pore-level liquid water transport through composite diffusion media of PEMFC", *J. Electrochem. Soc.* **157** (12) B1753−B1761 (2010).
3. Y. Wang, K. S. Chen, J. Mishler, S. C. Cho, and X. C. Adroher, "A Review of Polymer Electrolyte Membrane Fuel Cells: Technology, Applications, and Needs on Fundamental Research", *Applied Energy*, **88**, 981(2010).
4. Y. Wang and K. S. Chen, "Elucidating through-plane Liquid Water Profile in a Polymer Electrolyte Fuel Cell", in *ECS Transaction*, **33** (1) 1605-1614 (2010).
5. K. S. Chen, B. Carnes, F. Jiang, G. Luo, and C.-Y. Wang, "Toward developing a computational capability for PEM fuel cell design and optimization", in ASME Proceedings of FuelCell2010, paper #33037.
6. B. Carnes, K. S. Chen, F. Jiang, G. Luo, and C.-Y. Wang, "Systematic parameter estimation and sensitivity analysis using a multidimensional PEMFC model coupled with DAKOTA", in ASME Proceedings of FuelCell2010, paper #33038.
7. K. S. Chen, "Development and Validation of a Two-phase, Three-dimensional Model for PEM Fuel Cells", invited presentation at the 2010 LANL(US)/AIST-NEDO(Japan) Fuel Cell Workshop, Hyatt Regency Waikiki Beach Resort and Spa, Honolulu, HI, August 9 – 11, 2010.
8. K. S. Chen, "Development and Validation of a Two-phase, Three-dimensional Model for PEM Fuel Cells", presentation at the DOE Fuel Cell Tech Team July 14 Meeting, USCAR Office, Southfield, MI (2010).
9. F. Jiang, G. Luo, C.-Y. Wang, and K. S. Chen, "Simulation of a PEMFC with Zigzag Flow Field", presentation at the ASME 8th Int. Fuel Cell Sci., Eng. & Tech. Conf., Brooklyn, NY, June 14−16, 2010; paper #33108.
10. G. Luo, F. Jiang, C.-Y. Wang, and K. S. Chen, "Numerical Modeling of Micro-porous Layers in a Two-Phase Multidimensional PEM Fuel Cell Model", presentation at the ASME 8th International Fuel Cell Science, Engineering & Technology Conference, Brooklyn, NY, June 14−16, 2010; paper #33164.
11. Y. Ji, G. Luo, and C.-Y. Wang, "Computer Simulation of Liquid Water Transport at Pore Level in MPL and GDL and Their Interface", presentation at the ASME 8th International Fuel Cell Science, Engineering & Technology Conference, Brooklyn, NY, June 14−16, 2010; paper #33122.