SAND 2011-1887C

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

Ken S. Chen (PI)

Sandia National Laboratories

May 12, 2011

FC027

Overview

Sandia National Laboratories

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;

  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).

* 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.
- 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.

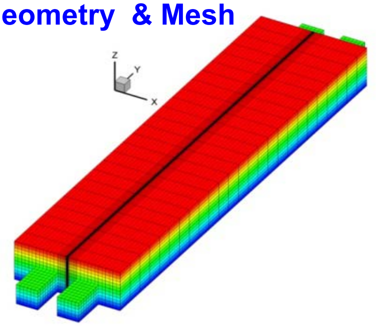
Approach

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

Geometry & 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

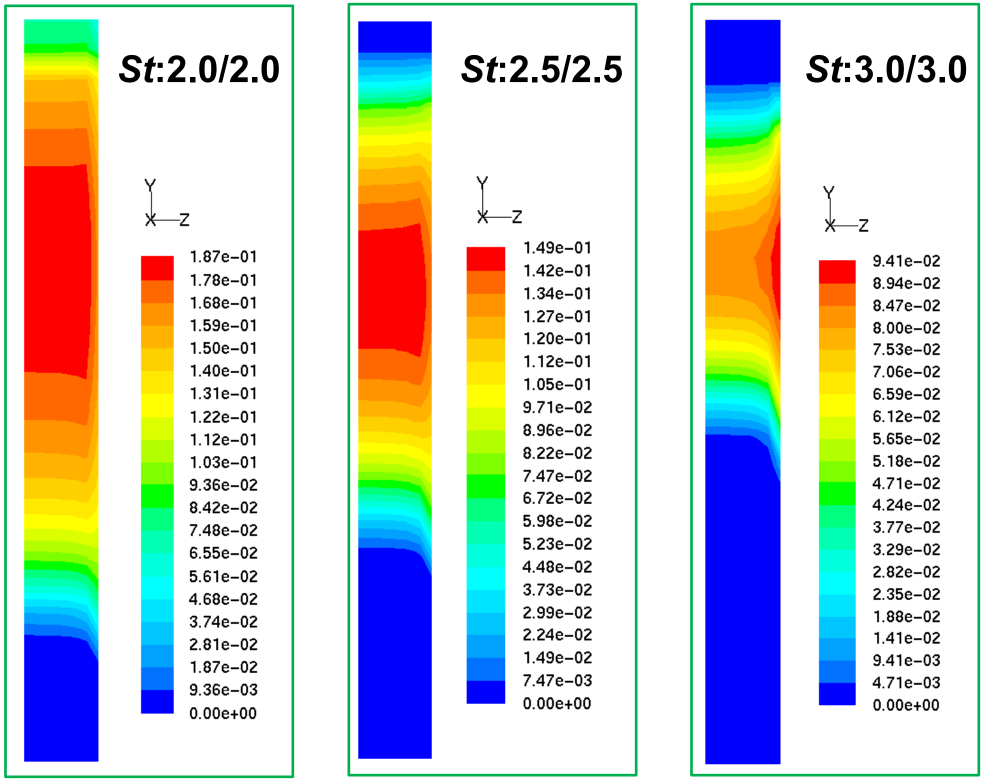
Operating Conditions: (Counter flow)

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

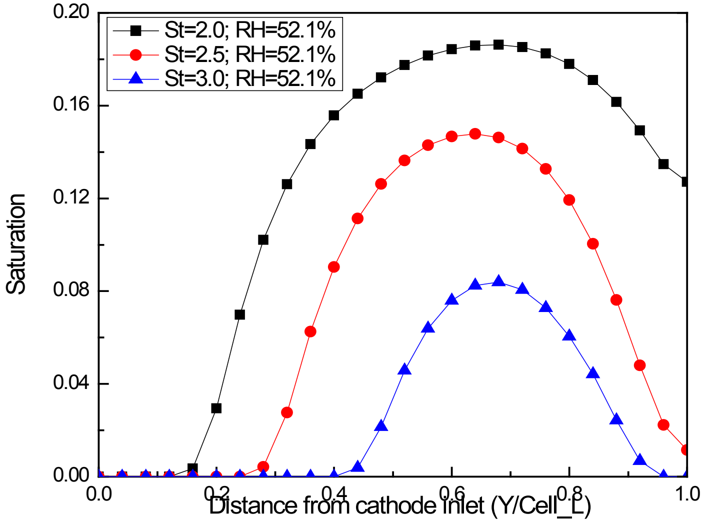
Inlet %*RH*(a/c)= 52.1/52.1

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

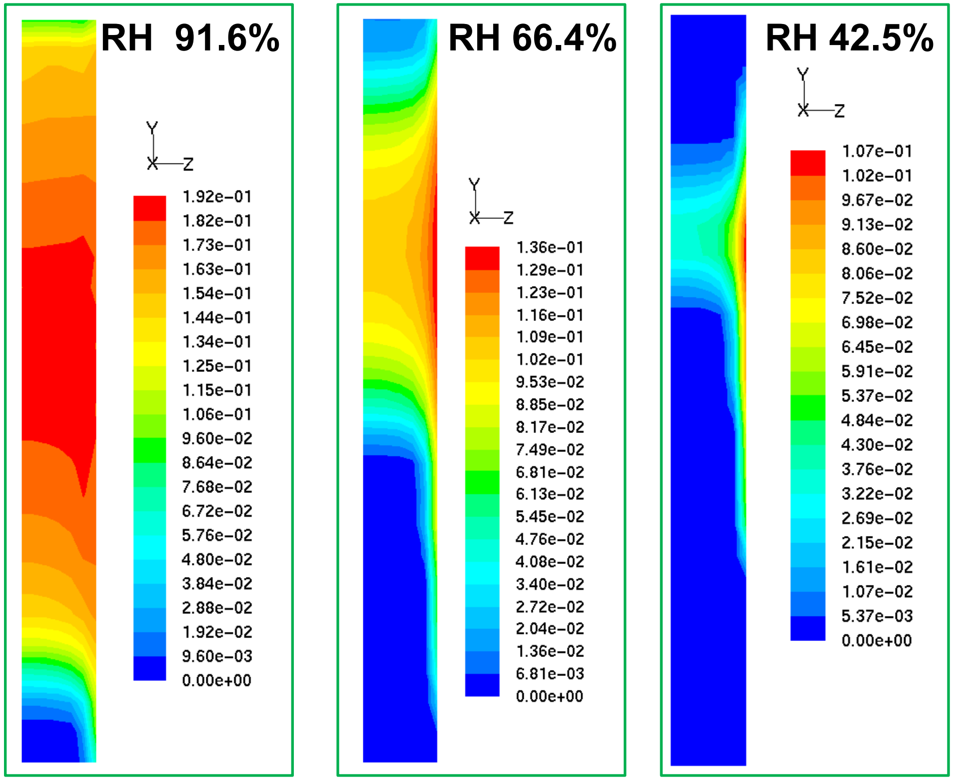
Operating Conditions: (Counter flow)

I= <u>0.8 A/cm^2</u> T_{cell} =<u>80 ^{o}C</u> P_a=P_c= <u>200kPa</u>

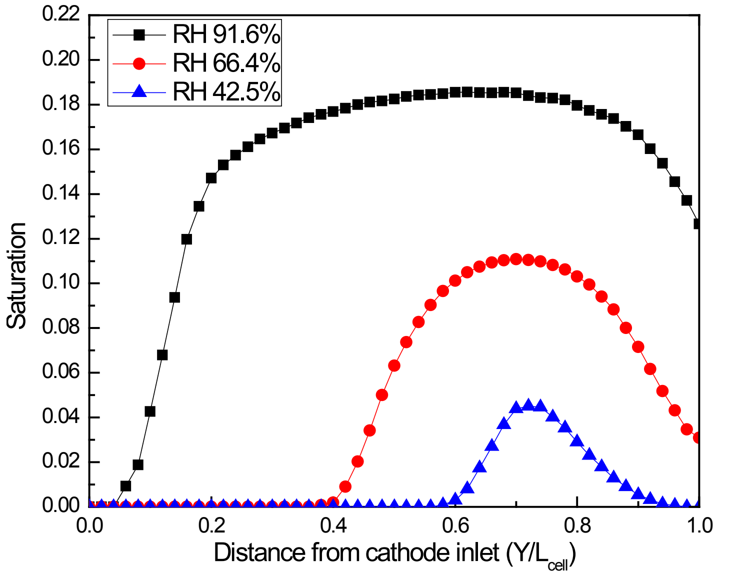
St(a/c) (H_2/air) = <u>1.8/2.0</u>

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

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

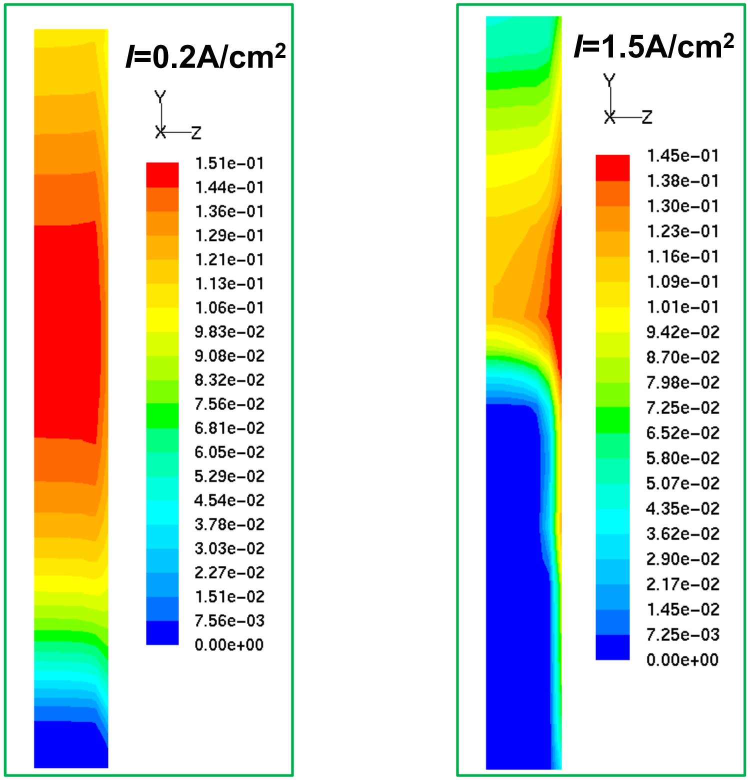
Operating Conditions: (Counter flow)

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

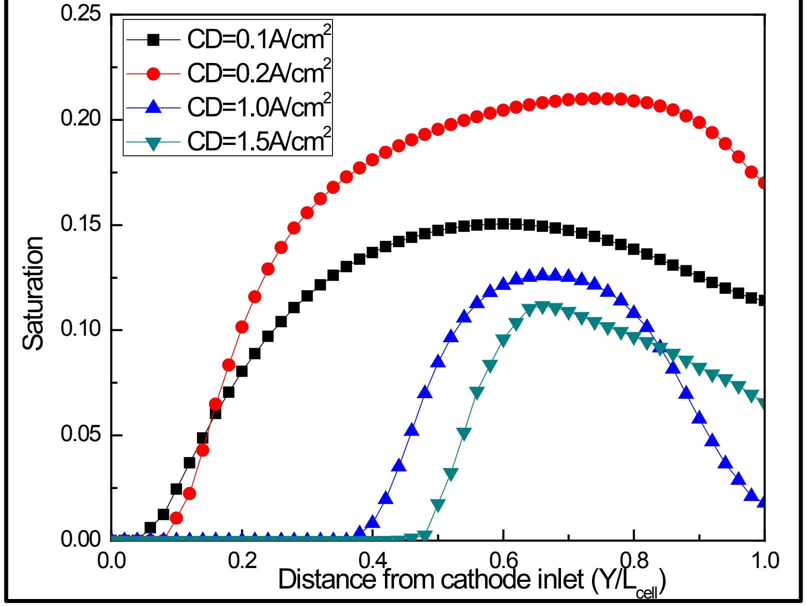
P_a=P_c= 200kPa *St*(a/c) (H_2/air) = 1.8/2.0

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

Liquid saturation at cathode GFC/GDL interface

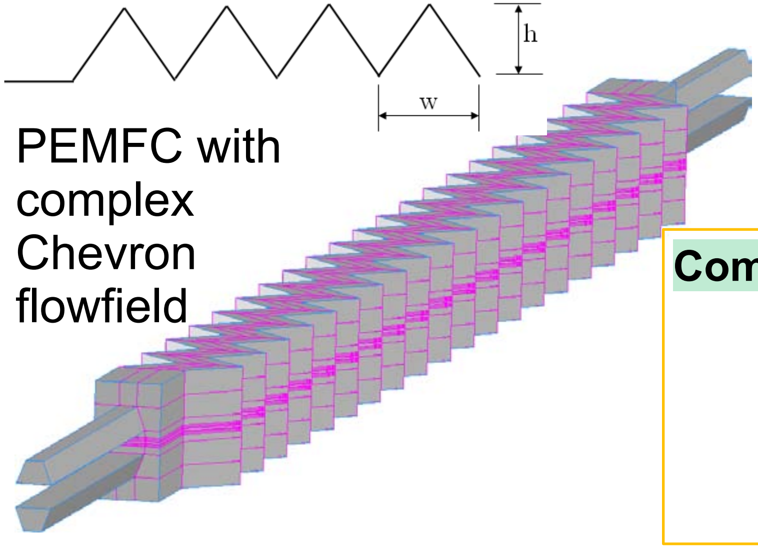


Liquid saturation along cathode channel with various current densities



- ❖ 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



PEMFC with complex Chevron flowfield

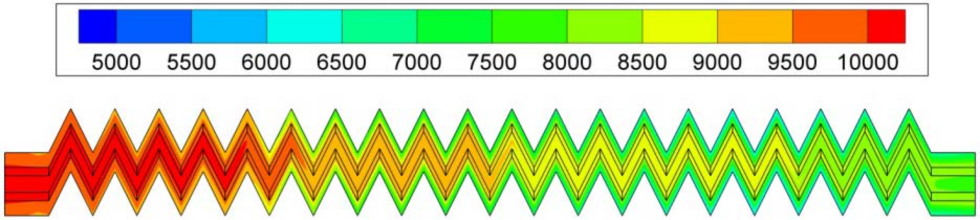
Operating Conditions and geometry (Counter flow)

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

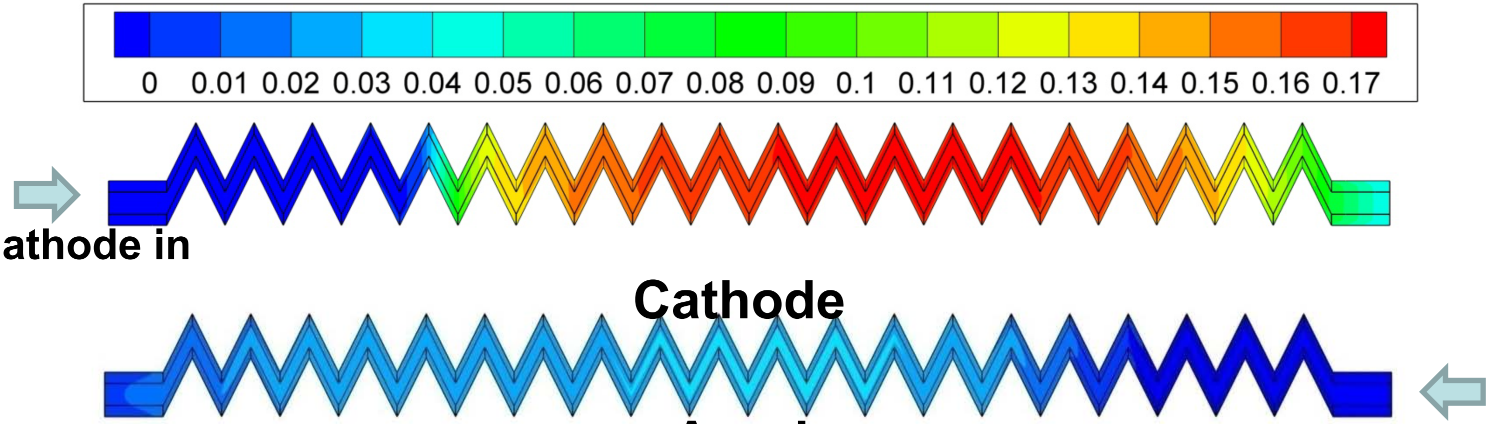
P_a=P_c= 200 kPa   Inlet %RH(a/c)= 81.4/81.4

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

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

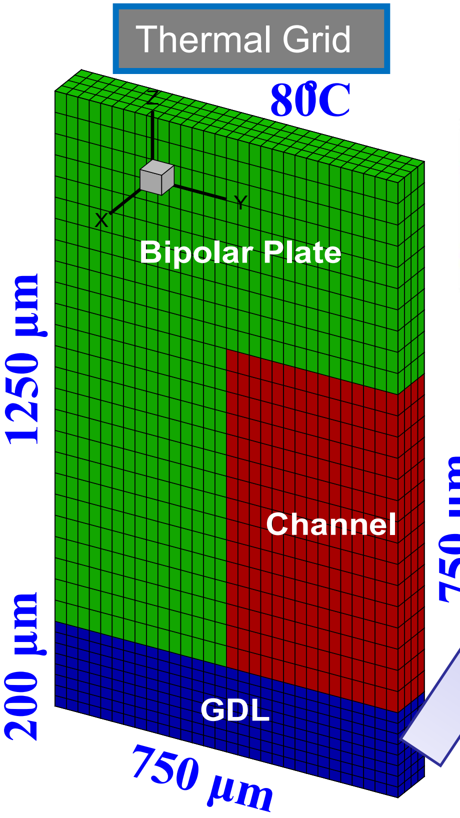


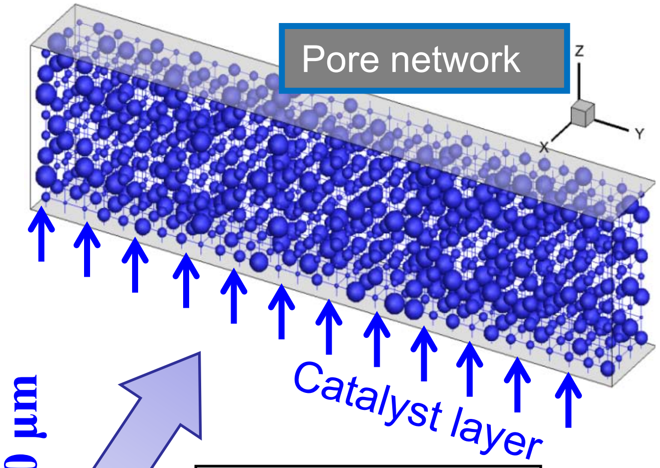
Computed liquid-water saturation along gas flow channel



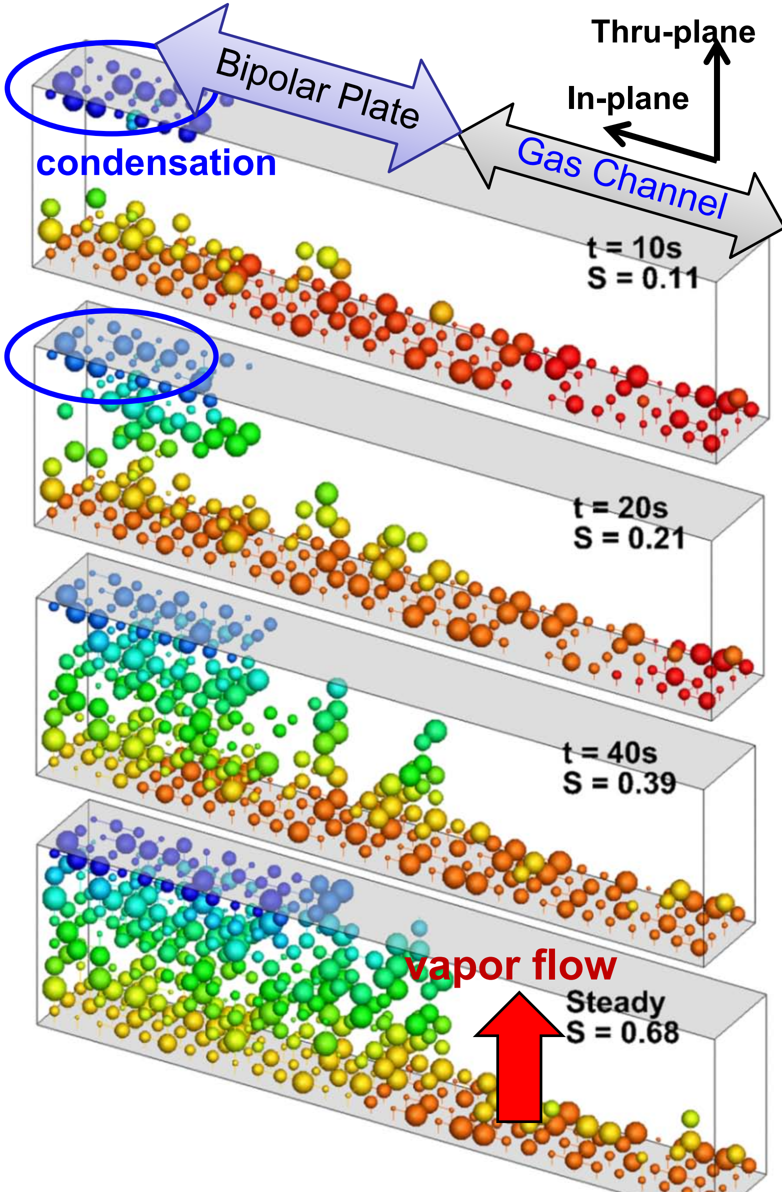
The present model is capable of simulating PEMFC with complex flowfield!

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





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

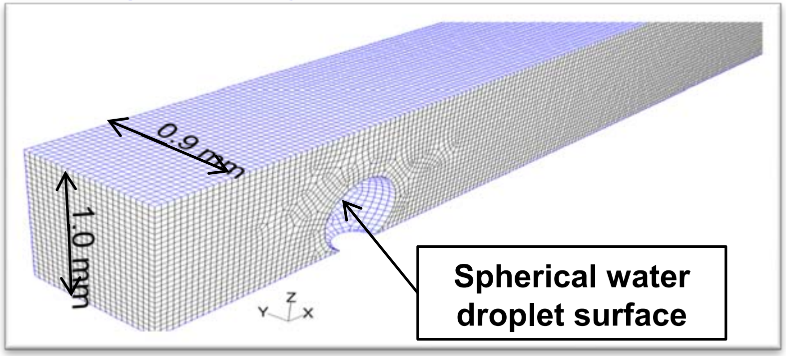


Model Capabilities:
- Heat transfer in pores & solid matrix
- Water vapor diffusion in the pores
- Phase change rates (diffusion limited) & location
- Capillary dominated drainage (invasion & condensation)
- Capillary dominated imbibition (evaporation)

Technical Accomplishment:

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

Model geometry for 3-D CFD simulation

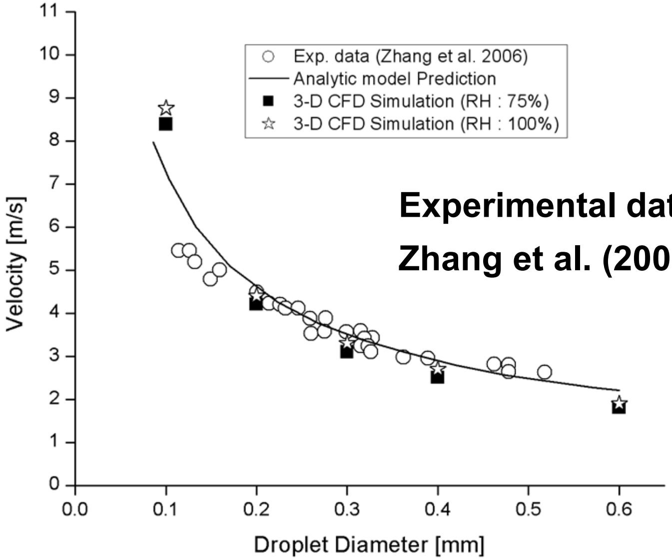


Spherical water droplet surface

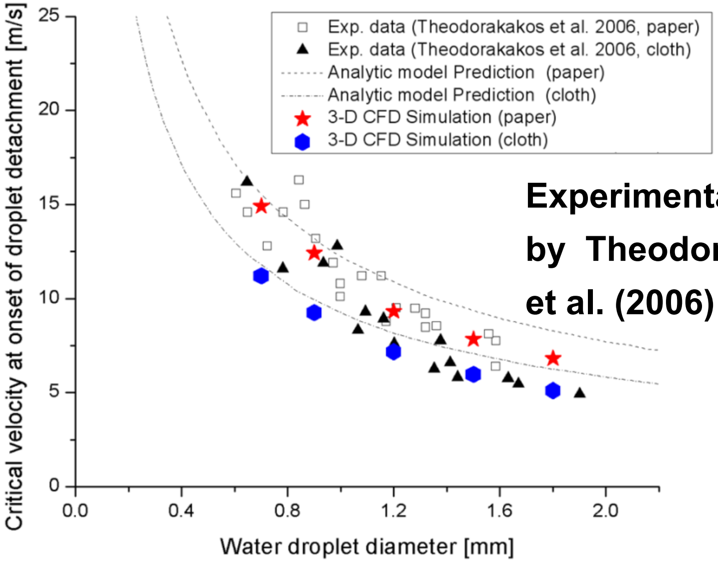
Analytical model: detachment velocity as a function of droplet size (Chen 2008)

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

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



Experimental data by Zhang et al. (2006)



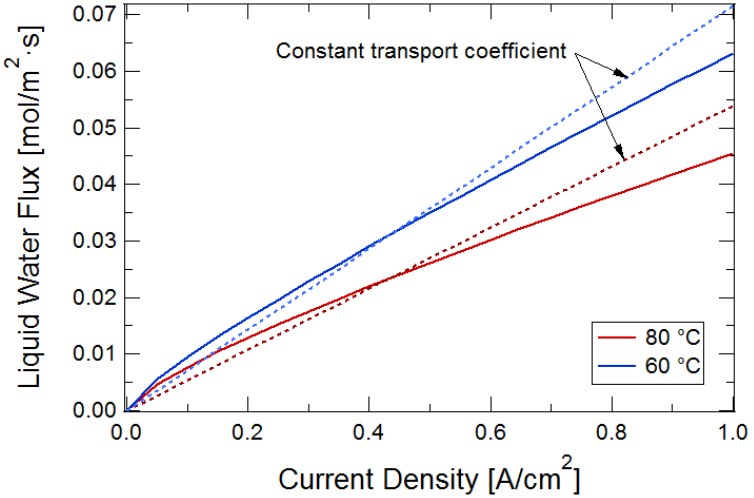
Experimental data by Theodorakakos et al. (2006)

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]

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

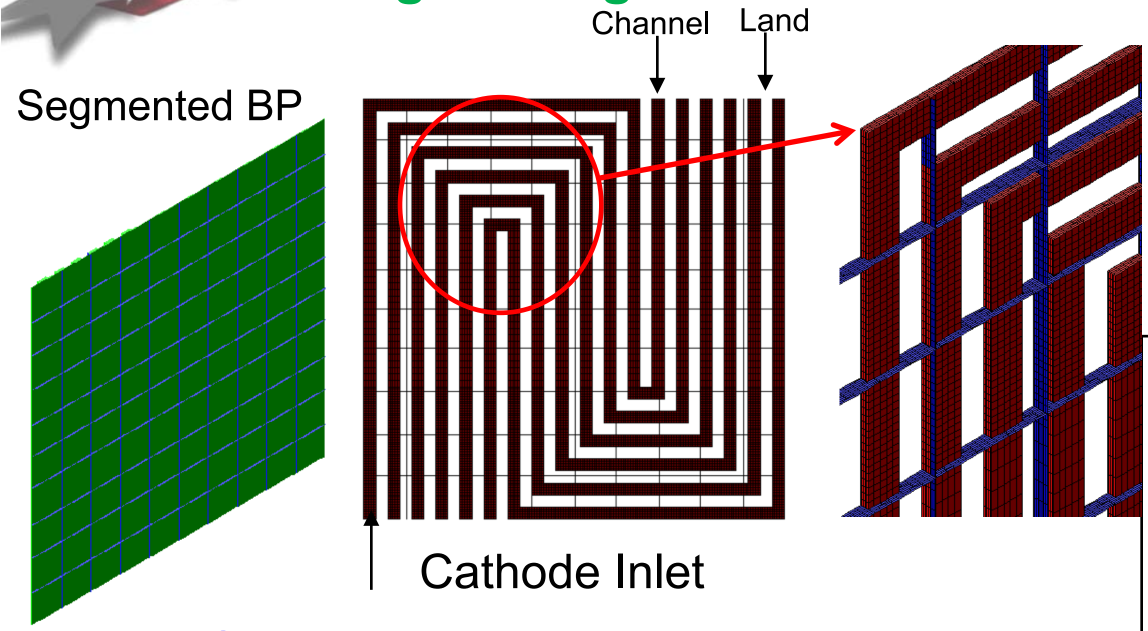
$$\beta = 0.2191\, i^{-0.374}, \text{ where } i \text{ is in A/cm}^2 \quad [3]$$

[1] A.Z. Weber, M.A. Hickner, *Electrochimica Acta* 53 (2008) 7668–7674.

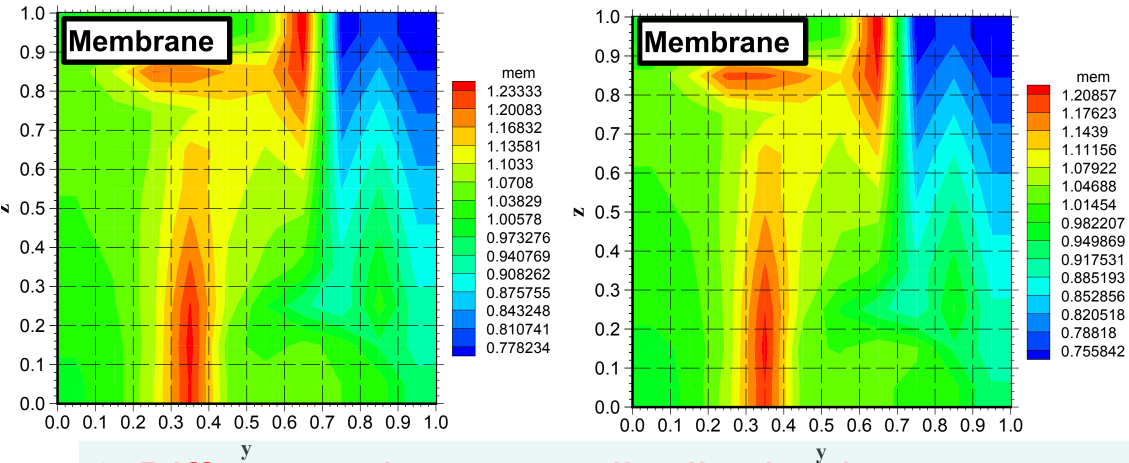
[2] K. S. Chen, *Proc. Int. Conf. on Fuel Cell Sci., Eng. & Tech.*, June 16–18, 2008, Denver, Colorado.

[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

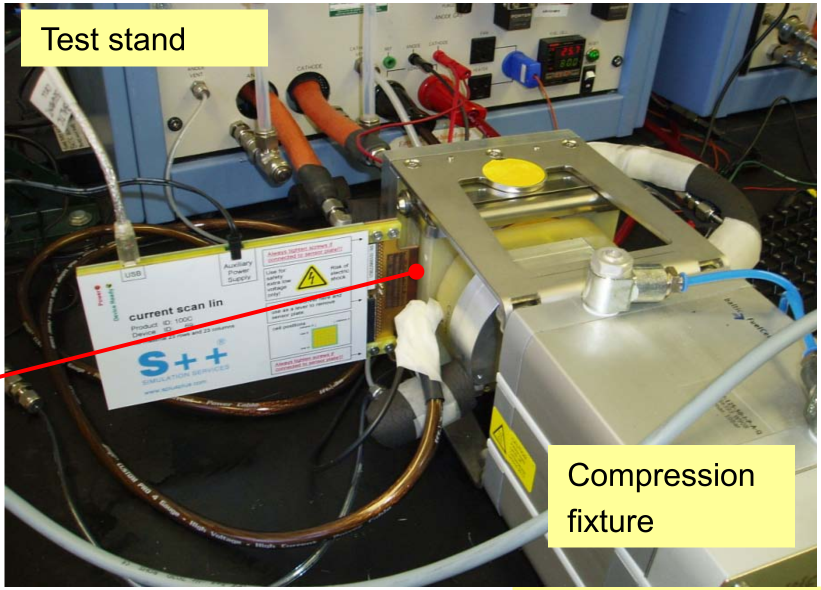
  2) Large errors seen mostly in U-turn regions where a segment contains mixed and irregular types of regions with flow channels and lands.

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

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

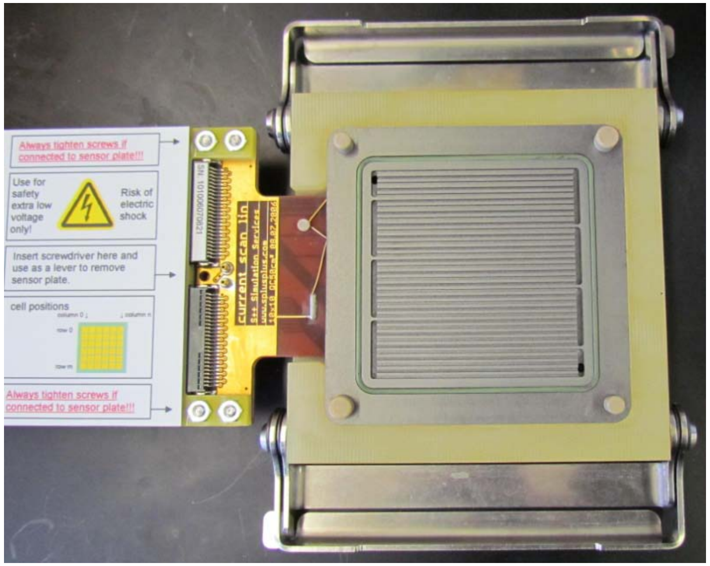
Fuel Cell Assembly 50 cm^2
- Current and T Distribution (10 x 10 segments)
- Varying Compression

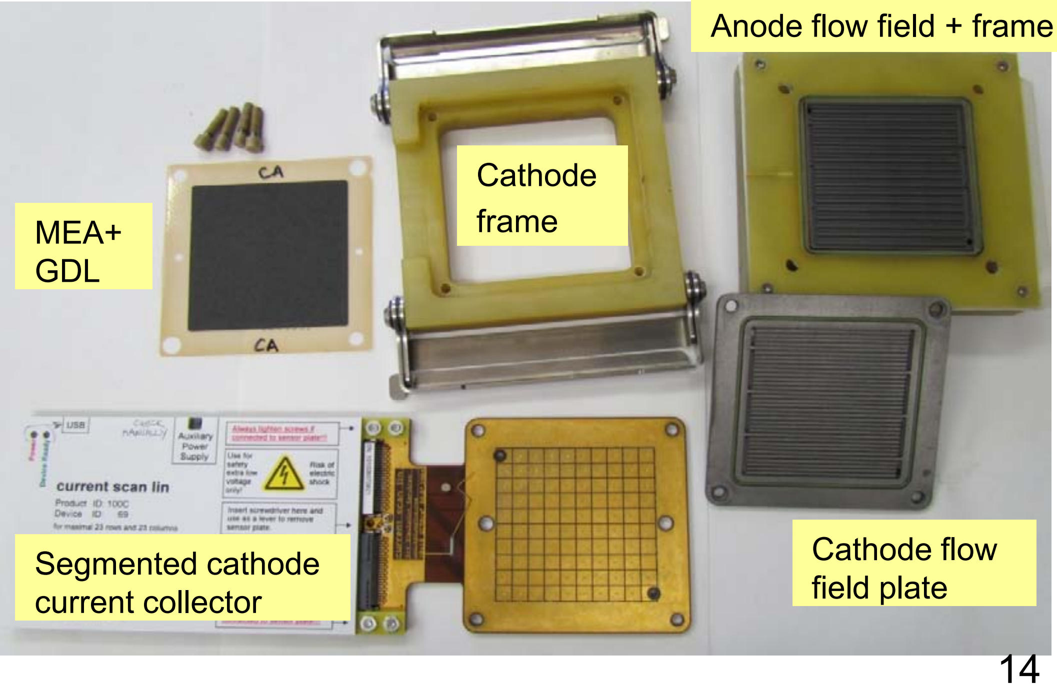
Assembled fuel cell
w. segmented current collector


Test stand

Compression fixture

Assembled cathode side:
flow field + frame + current collector




Anode flow field + frame

MEA+
GDL

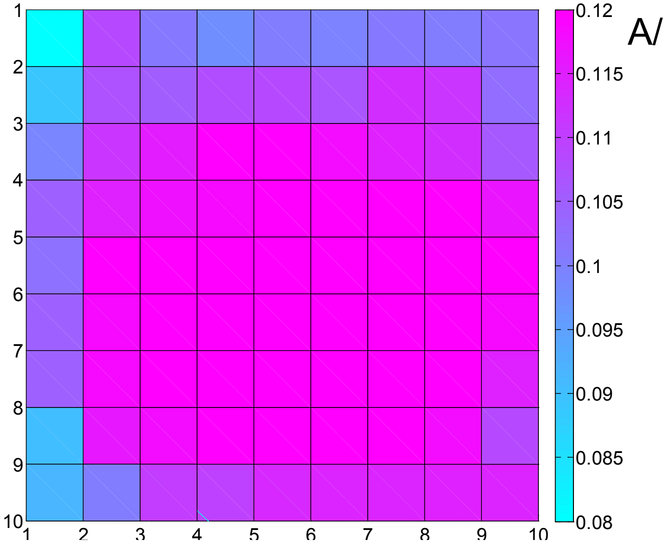
Cathode
frame

Segmented cathode
current collector

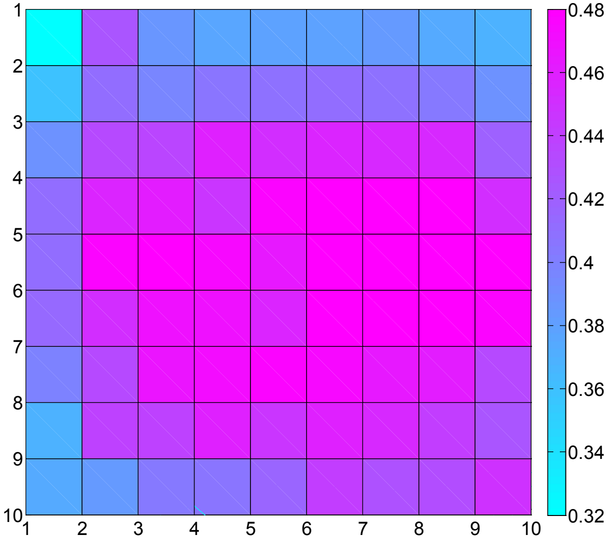
Cathode flow
field plate

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

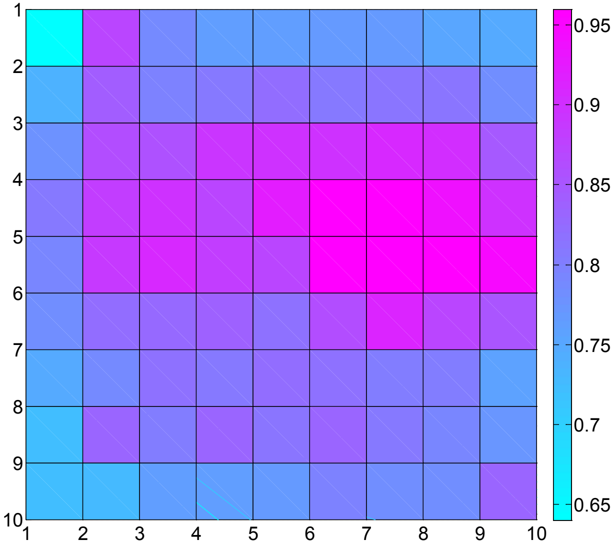
Cell Area = 50 cm^2, Flow Field = 5-pass serpentine with manifolds, Segmented Current Collector = 10 x10 segments
MEA (catalyst coated membrane) = A510.2/M710.18/C510.4 (by W. L. Gore), GDL = SGL24BC (by SGL Carbon)
GDL – 200μm, MPL – 50μm, cathode CL – 20μm, anode CL – 10μm, membrane – 18μm.



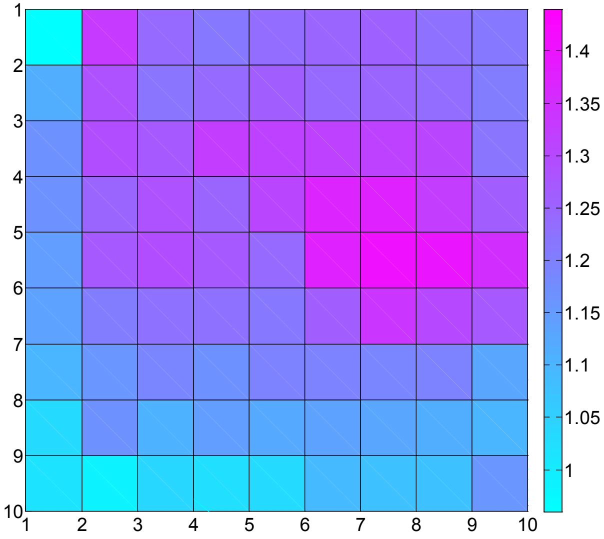
I = 0.1 A/cm^2



I = 0.4 A/cm^2



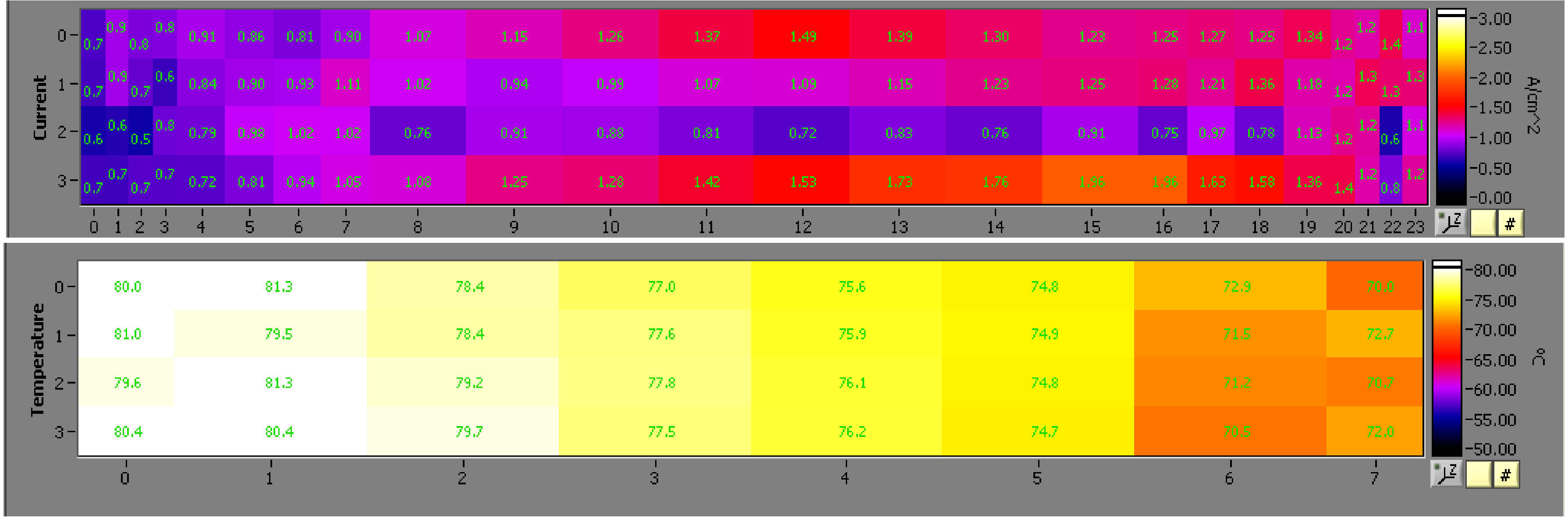
I = 0.8 A/cm^2



I = 1.2 A/cm^2

Technical Accomplishment: Simultaneous current & temperature distribution measurements

Ballard’s current and temperature mapping tool



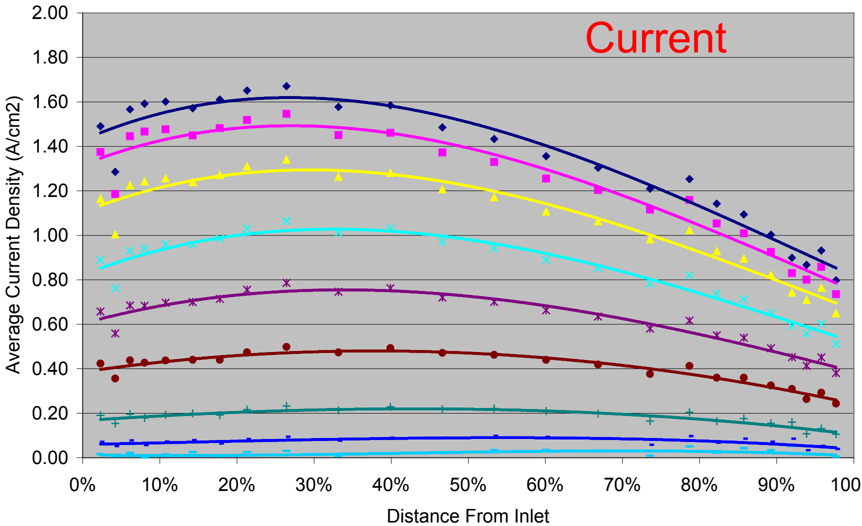
Current

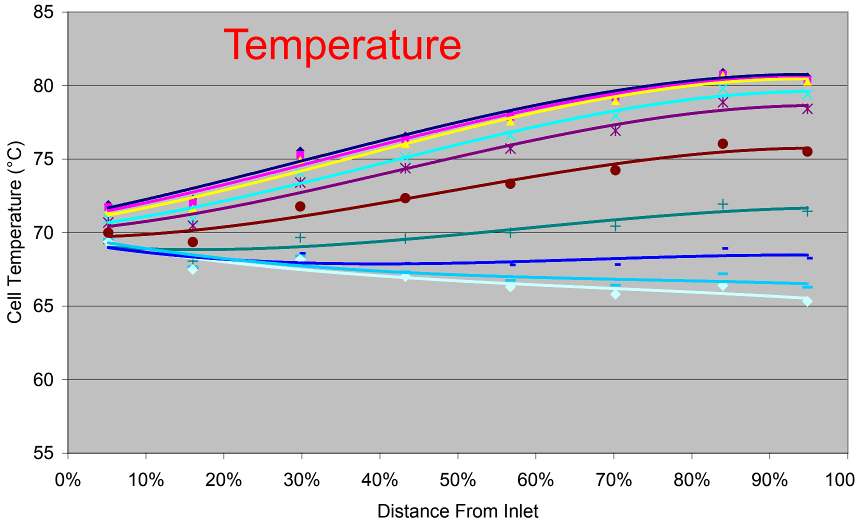
	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23
0	0.7	0.9	0.8	0.8	0.91	0.86	0.81	0.90	1.07	1.15	1.26	1.37	1.49	1.39	1.30	1.23	1.25	1.27	1.25	1.34	1.2	1.2	1.4	1.1
1	0.7	0.9	0.7	0.6	0.84	0.90	0.93	1.11	1.02	0.94	0.99	1.07	1.09	1.15	1.23	1.25	1.28	1.21	1.36	1.18	1.2	1.3	1.3	1.3
2	0.6	0.6	0.5	0.8	0.79	0.98	1.02	1.02	0.76	0.91	0.88	0.81	0.72	0.83	0.76	0.91	0.75	0.97	0.78	1.13	1.2	1.2	0.6	1.1
3	0.7	0.7	0.7	0.7	0.72	0.81	0.94	1.05	1.08	1.25	1.28	1.42	1.53	1.73	1.76	1.96	1.96	1.63	1.58	1.36	1.4	1.2	0.8	1.2

Temperature

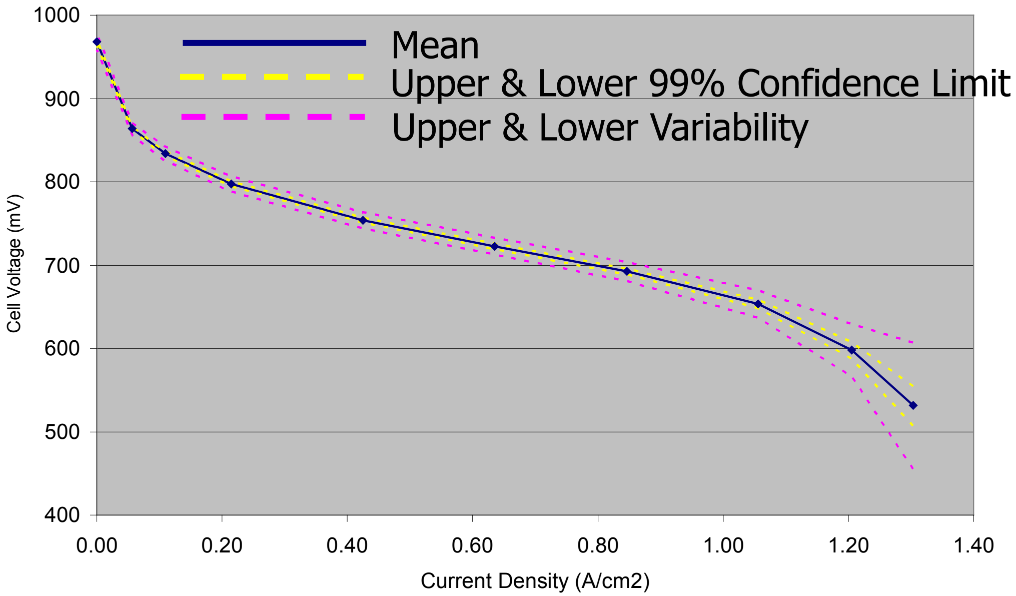
	0	1	2	3	4	5	6	7
0	80.0	81.3	78.4	77.0	75.6	74.8	72.9	70.0
1	81.0	79.5	78.4	77.6	75.9	74.9	71.5	72.7
2	79.6	81.3	79.2	77.8	76.1	74.8	71.2	70.7
3	80.4	80.4	79.7	77.5	76.2	74.7	70.5	72.0

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



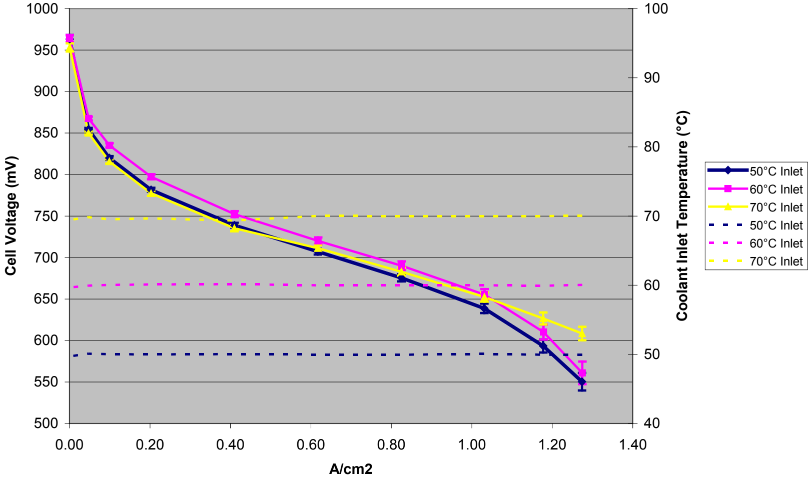


Technical Accomplishment: Polarization curves with upper and lower bounds (Ballard)

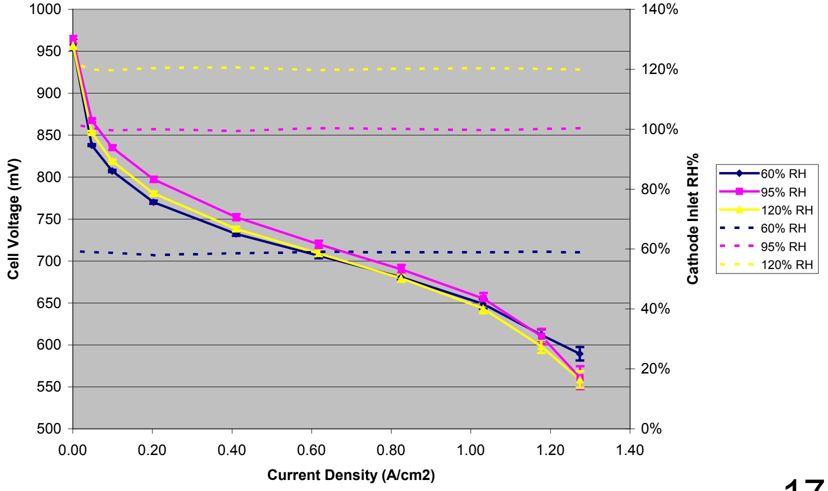


Sample polarization curve with upper and lower bounds

Temperature sensitivity



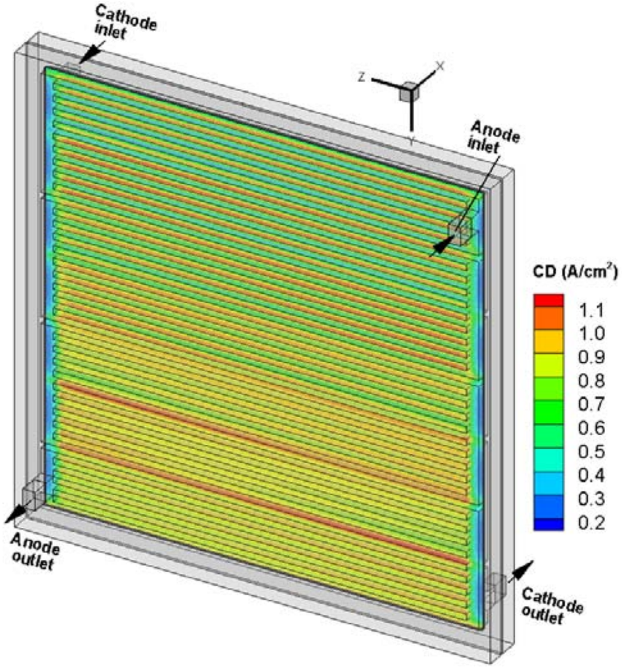
RH sensitivity



Validation Procedure

- 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 & 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

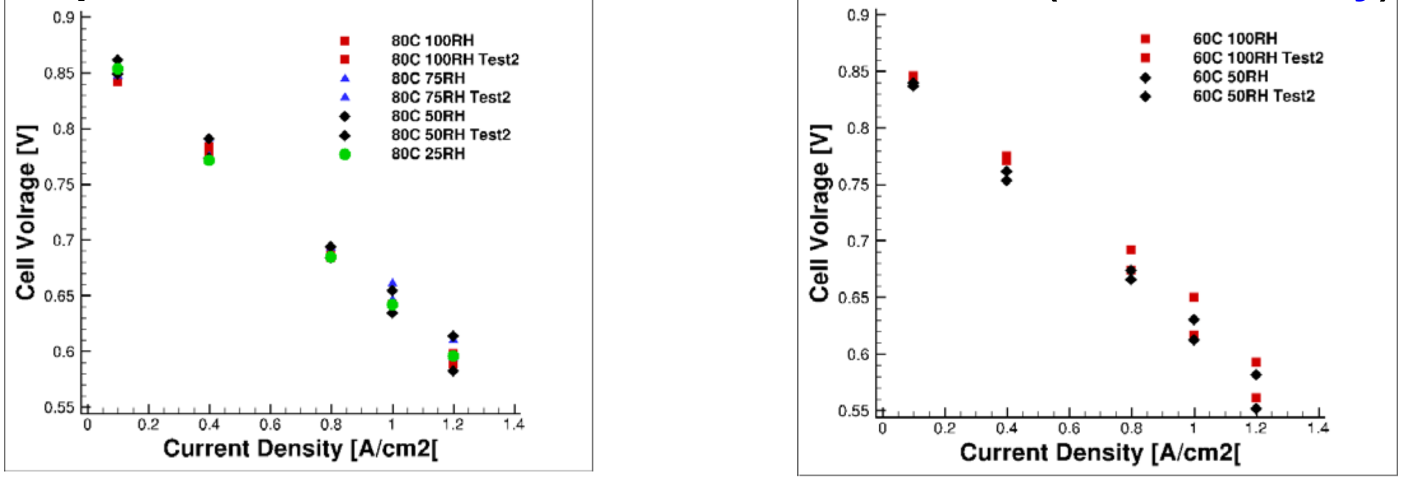
Predicted membrane current distribution



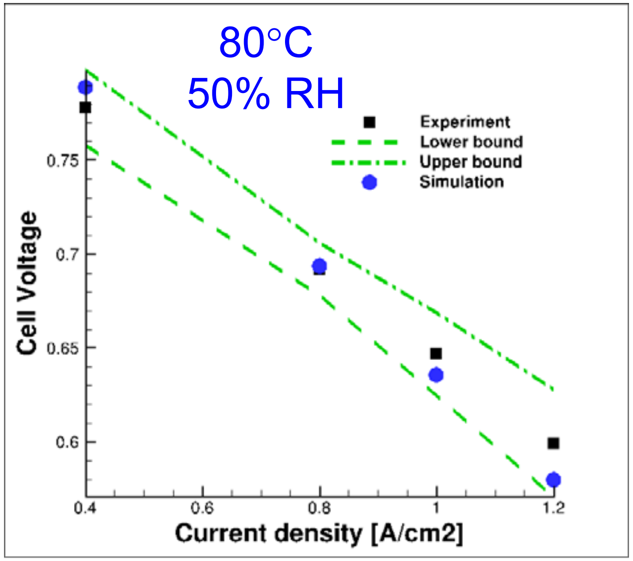
Operating conditions:
Stoich(a/c): 1.2/2
Pressure(a/c): 1.95 atm
Materials/geometry:
Gore MEA (18 μm mem.)
Pt (a/c): 0.2/0.4 mg/cm^2
Cell area: 50 cm^2

Technical Accomplishment:
Model Validation: I-V Curves

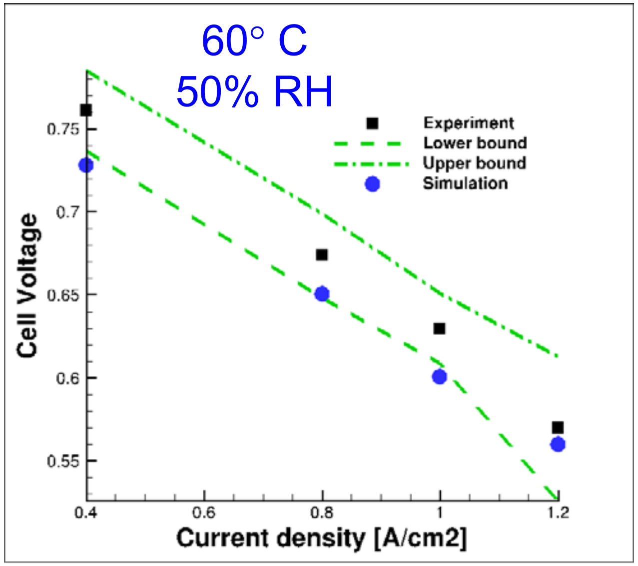
Experimental data from LANL at 80°C and 60°C (note variability)



80°C
50% RH



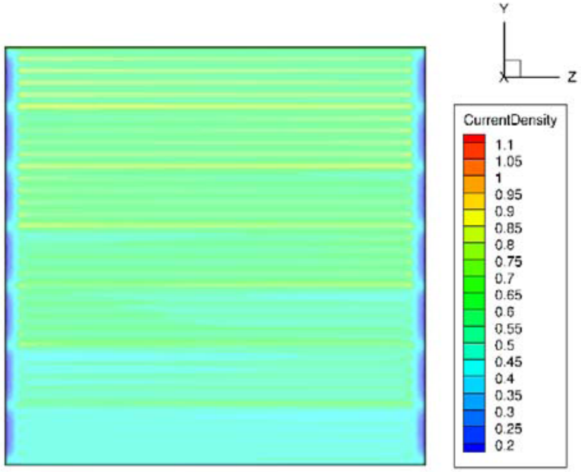
60° C
50% RH



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

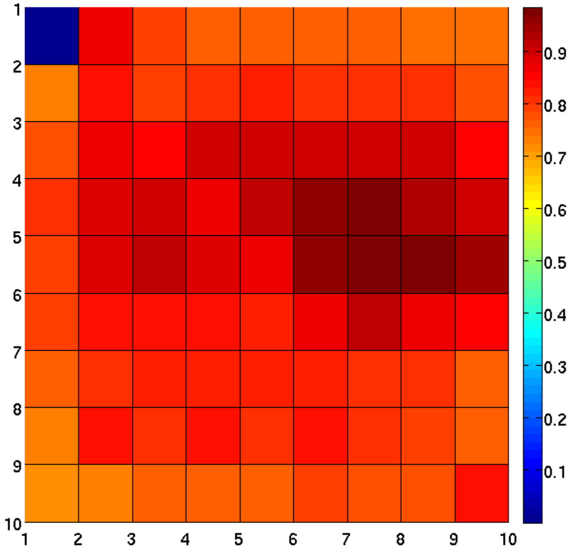
Technical Accomplishment: Validation: Current Distribution

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



Operating Conditions:
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

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

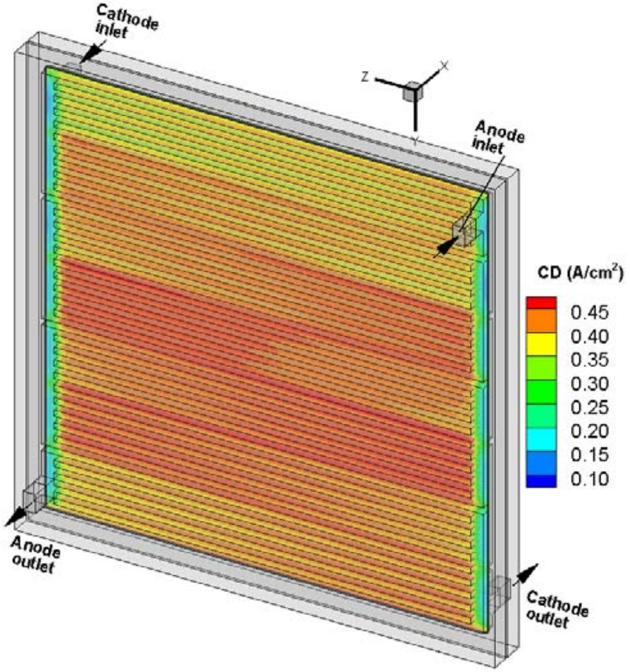
Experimental data

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

Predicted membrane current density distribution



Relative difference between experimental data and simulation

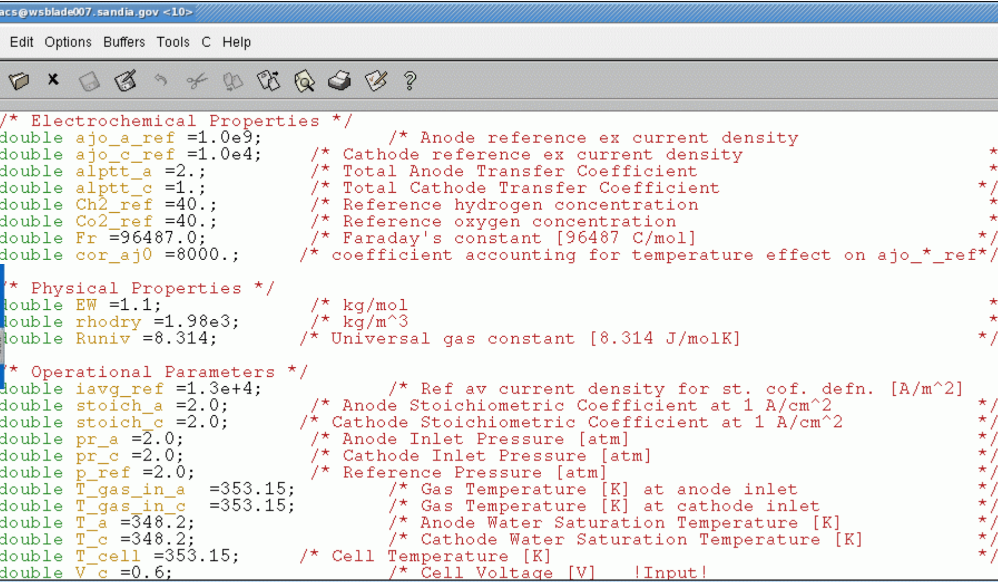
0.0%	15.3%	5.4%	2.1%	1.8%	1.4%	1.5%	-1.7%	-4.5%	8.8%
7.9%	4.7%	0.9%	4.0%	4.2%	4.7%	4.6%	3.3%	-0.4%	13.4%
11.4%	5.3%	6.7%	11.7%	11.0%	12.1%	12.2%	13.0%	6.4%	19.7%
19.7%	11.6%	11.6%	7.9%	13.0%	16.6%	16.4%	11.5%	5.4%	19.3%
12.7%	9.4%	11.2%	9.1%	7.1%	15.2%	18.8%	19.4%	14.3%	24.0%
12.1%	2.9%	6.8%	7.2%	4.8%	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%!

PEMFC Model Demo: Overview of code and files

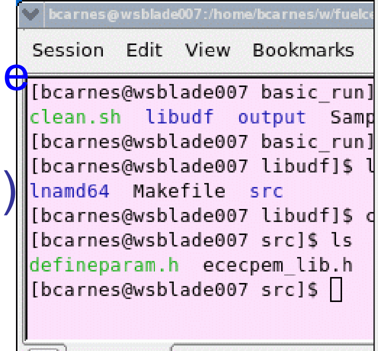
- The code is based on FLUENT with extensive user-defined functions (UDF) to provide additional capability.
- Prerequisites for the code are
  - the *.cas file (“Sample.cas”)
  - the UDF library (“libudf”)
  - an installation of FLUENT and C compiler
- Contents of the Sample.cas file
  - The computational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

Setting input parameters

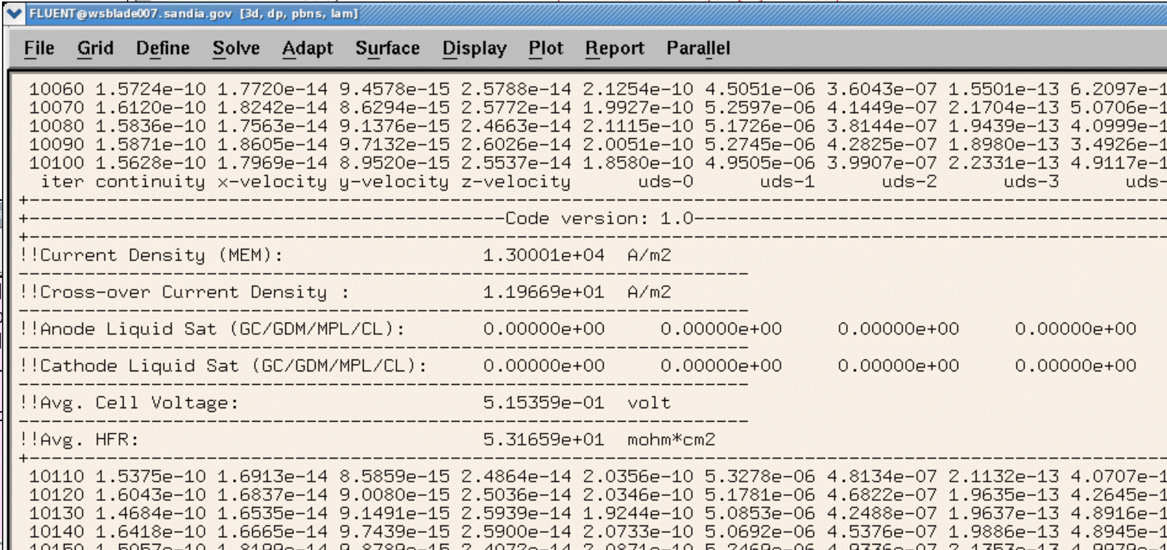


```
/* Electrochemical Properties */
double ajo_a_ref =1.0e9;              /* Anode reference ex current density
double ajo_c_ref =1.0e4;       /* Cathode reference ex current density               *
double alptt_a =2.;            /* Total Anode Transfer Coefficient                   *
double alptt_c =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_*_ref*/

/* 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!
```

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



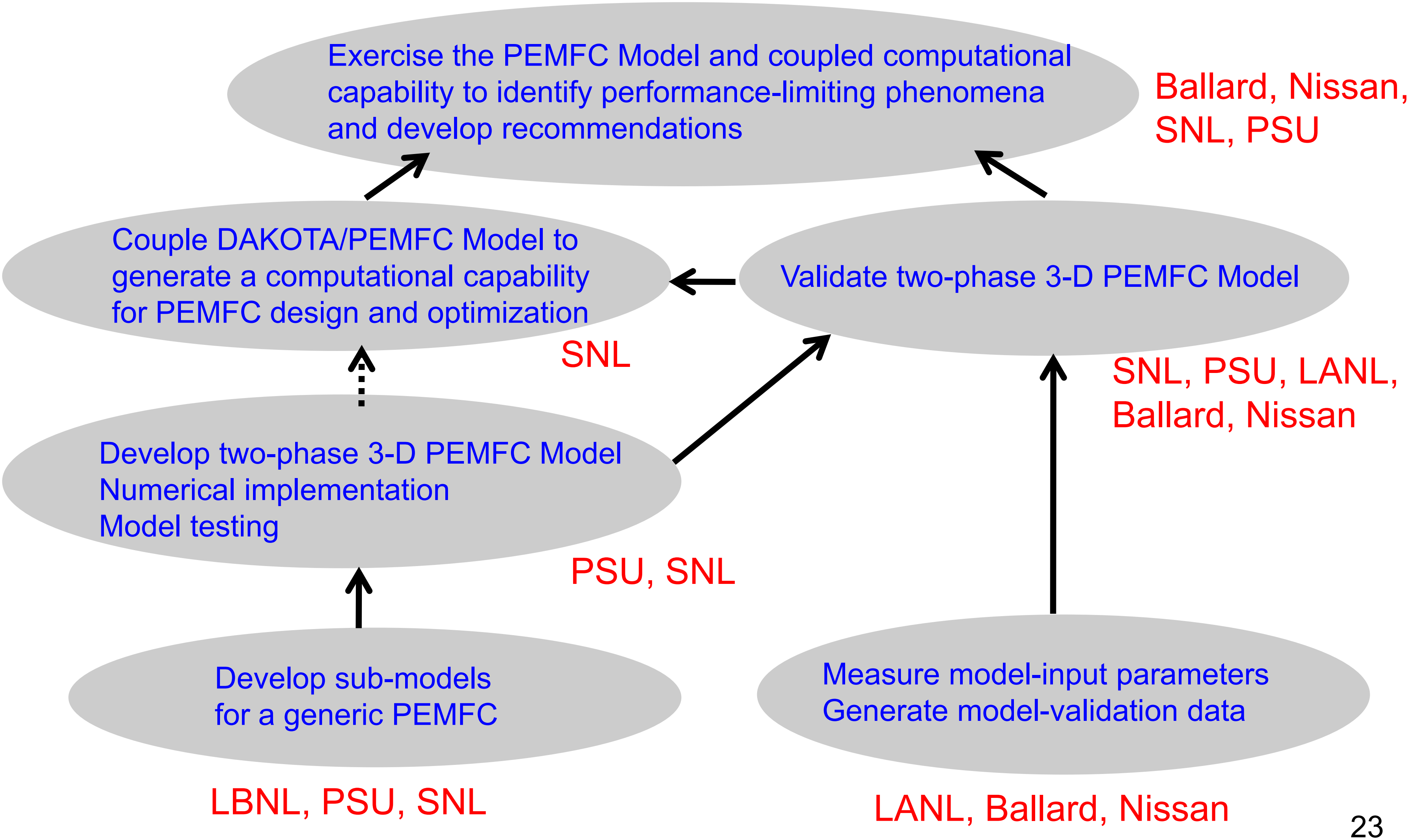
```
[bcarnes@wsblade007 basic_run]
clean.sh  libudf  output  Samp
[bcarnes@wsblade007 basic_run]
[bcarnes@wsblade007 libudf]$ l
lnamd64  Makefile  src
[bcarnes@wsblade007 libudf]$ c
[bcarnes@wsblade007 src]$ ls
defineparam.h  ececpem_lib.h
[bcarnes@wsblade007 src]$ 
```



```
 10060 1.5724e-10 1.7720e-14 9.4578e-15 2.5788e-14 2.1254e-10 4.5051e-06 3.6043e-07 1.5501e-13 6.2097e-1
 10070 1.6120e-10 1.8242e-14 8.6294e-15 2.5772e-14 1.9927e-10 5.2597e-06 4.1449e-07 2.1704e-13 5.0706e-1
 10080 1.5836e-10 1.7563e-14 9.1376e-15 2.4663e-14 2.1115e-10 5.1726e-06 3.8144e-07 1.9439e-13 4.0999e-1
 10090 1.5871e-10 1.8605e-14 9.7132e-15 2.6026e-14 2.0051e-10 5.2745e-06 4.2825e-07 1.8980e-13 3.4926e-1
 10100 1.5628e-10 1.7969e-14 8.9520e-15 2.5537e-14 1.8580e-10 4.9505e-06 3.9907e-07 2.2331e-13 4.9117e-1
  iter continuity x-velocity y-velocity z-velocity      uds-0      uds-1      uds-2      uds-3      uds-
+---------------------------------------------------------------------------------------------------------
+-----------------------------------------Code version: 1.0-----------------------------------------------
+---------------------------------------------------------------------------------------------------------
!!Current Density (MEM):                1.30001e+04  A/m2
----------------------------------------------------------------
!!Cross-over Current Density :          1.19669e+01  A/m2
----------------------------------------------------------------
!!Anode Liquid Sat (GC/GDM/MPL/CL):     0.00000e+00     0.00000e+00     0.00000e+00     0.00000e+00
----------------------------------------------------------------
!!Cathode Liquid Sat (GC/GDM/MPL/CL):   0.00000e+00     0.00000e+00     0.00000e+00     0.00000e+00
----------------------------------------------------------------
!!Avg. Cell Voltage:                    5.15359e-01  volt
----------------------------------------------------------------
!!Avg. HFR:                             5.31659e+01  mohm*cm2
+---------------------------------------------------------------------------------------------------------
 10110 1.5375e-10 1.6913e-14 8.5859e-15 2.4864e-14 2.0356e-10 5.3278e-06 4.8134e-07 2.1132e-13 4.0707e-1
 10120 1.6043e-10 1.6837e-14 9.0080e-15 2.5036e-14 2.0346e-10 5.1781e-06 4.6822e-07 1.9635e-13 4.2645e-1
 10130 1.4684e-10 1.6535e-14 9.1491e-15 2.5939e-14 1.9244e-10 5.0853e-06 4.2488e-07 1.9637e-13 4.8916e-1
 10140 1.6418e-10 1.6665e-14 9.7439e-15 2.5900e-14 2.0733e-10 5.0692e-06 4.5376e-07 1.9886e-13 4.8945e-1
```

Collaborations

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



Exercise the PEMFC Model and coupled computational capability to identify performance-limiting phenomena and develop recommendations

Ballard, Nissan, SNL, PSU

Couple DAKOTA/PEMFC Model to generate a computational capability for PEMFC design and optimization

SNL

Validate two-phase 3-D PEMFC Model

SNL, PSU, LANL, Ballard, Nissan

Develop two-phase 3-D PEMFC Model
Numerical implementation
Model testing

PSU, SNL

Develop sub-models for a generic PEMFC

LBNL, PSU, SNL

Measure model-input parameters
Generate model-validation data

LANL, Ballard, Nissan

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 to address technical barriers & 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

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:

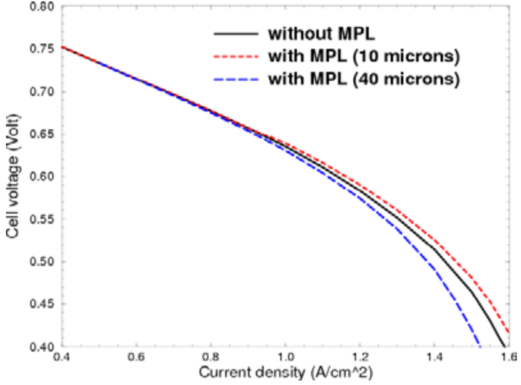
$$K_{MPL-GDL} = \frac{1}{\frac{1}{K_{MPL}} \frac{H_{MPL}}{H_{MPL}+H_{GDL}} + \frac{1}{K_{GDL}} \frac{H_{GDL}}{H_{MPL}+H_{GDL}}}$$

From capillary-pressure being additive:

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

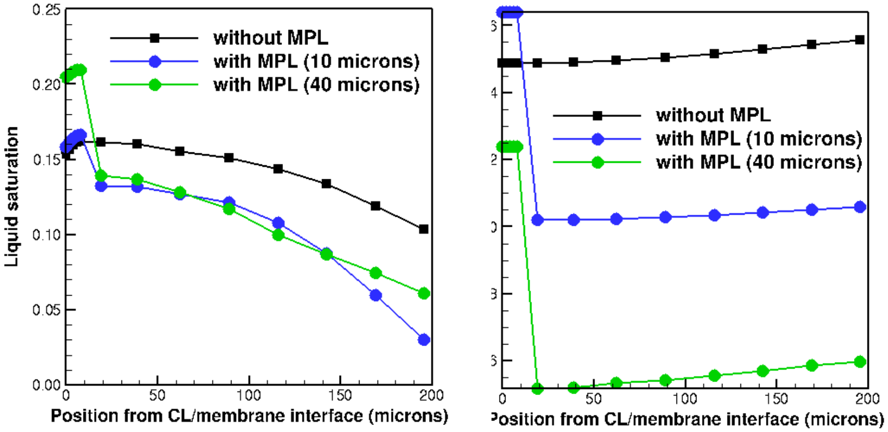
Parameters: $\varepsilon_{GDL} = 0.6$, $K_{GDL} = 10^{-12}\ m^2$, $\theta_{c,GDL} = 92^o$, $\varepsilon_{MPL} = 0.4$, $K_{MPL} = 10^{-13}\ m^2$, $\theta_{c,MPL} = 150^o$, $H_{GDL} + H_{MPL} = 200\ \mu m$

Computed effect of MPL on cell performance



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

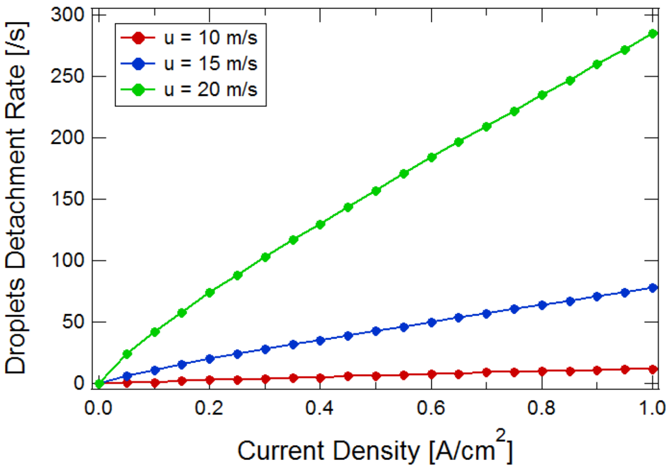
Computed liquid saturation across CL and MPL/GDL



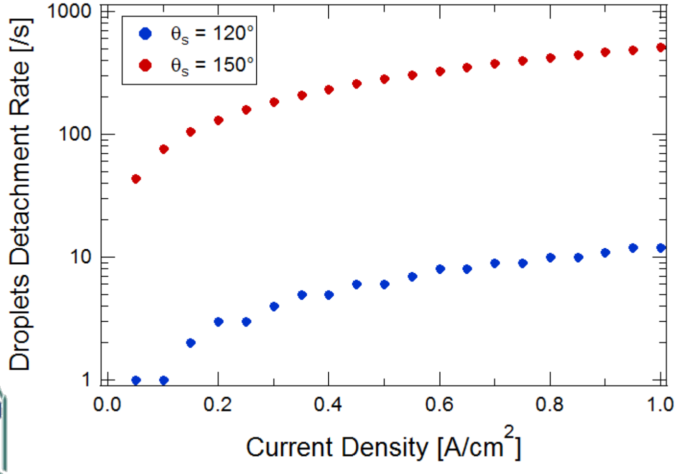
Incorporating hydrophobic MPL reduces liquid saturation in MPL/GDL, particularly under the land!

Back-of-Envelope Calculation: Droplets

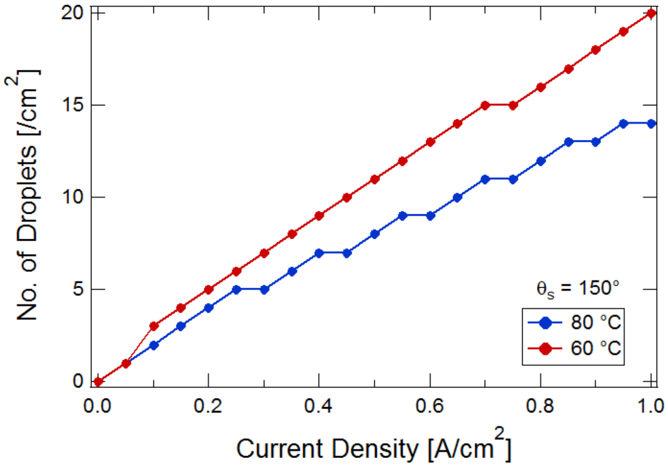
- Droplet detachment
  - Gas flow velocity



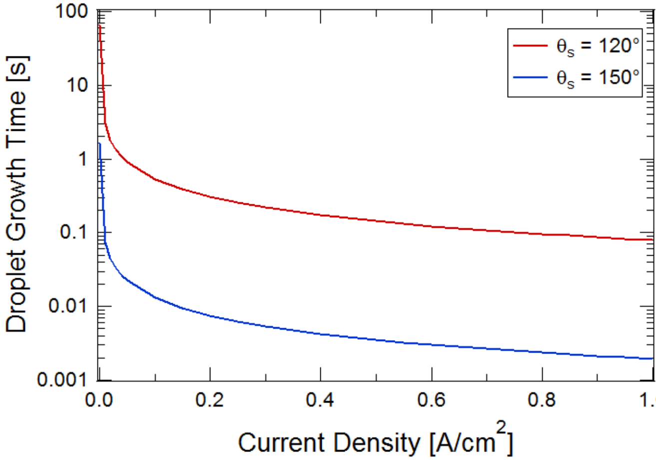
  - Surface static contact angle



- Droplets on surface
  - Number of droplets



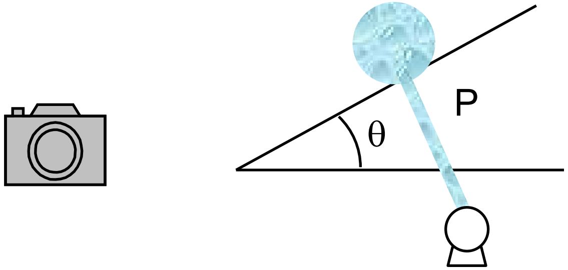
  - Growth of droplets



Droplet Imaging Experiment

Goal: Improve models and understand droplet governing physics

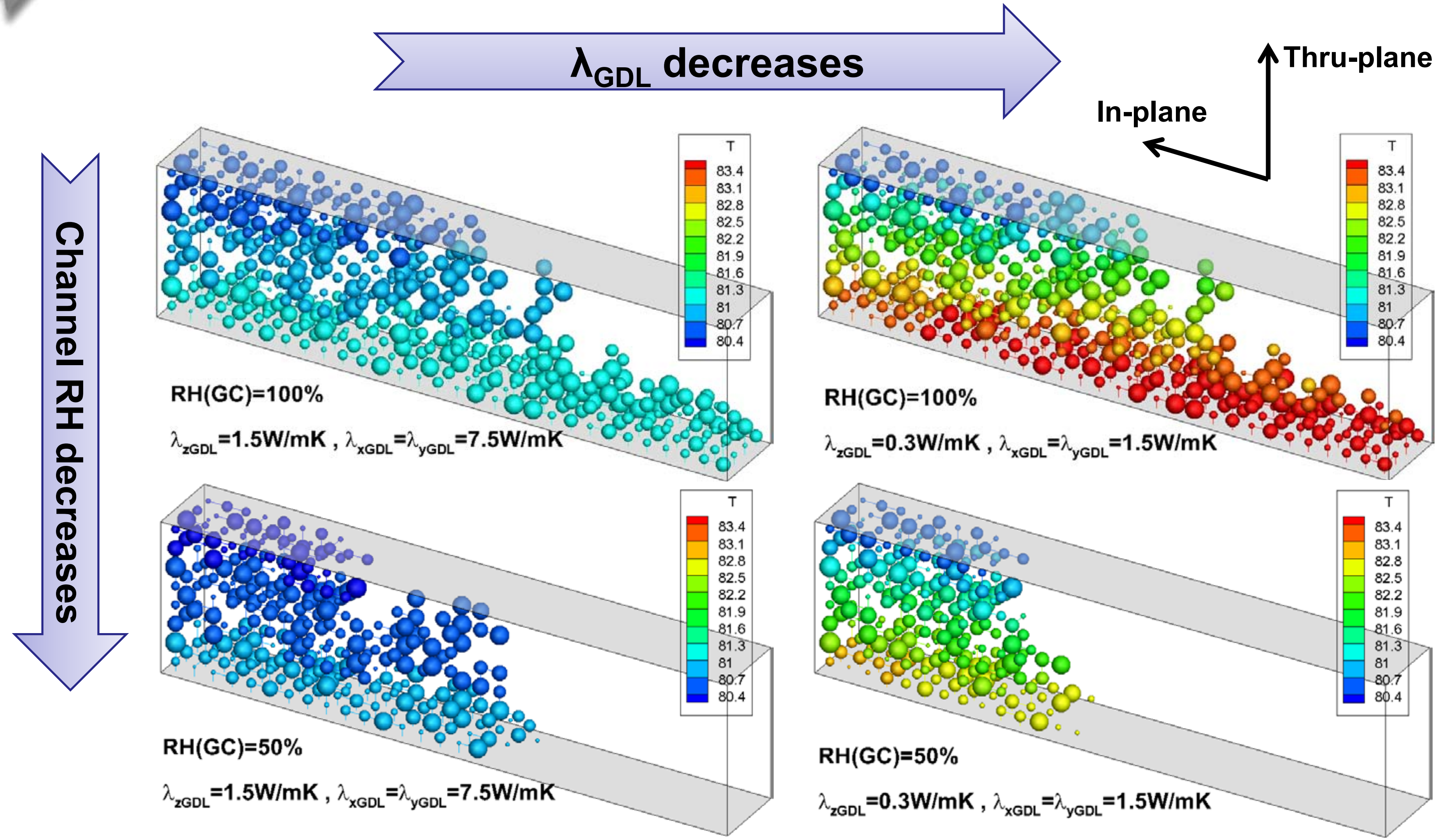
- Directly measure the adhesion force instead of depending on contact-angle measurements and hysteresis
  - Measure angle at which droplet begins to move and liquid pressure
- Measure real and ideal materials with liquid water injected



  - 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

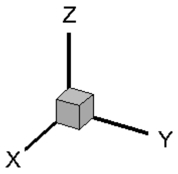
Goniometer with Tilt Stage

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


λ_{GDL} decreases

Channel RH decreases

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



Sensitivity Analysis Using PEMFC/DAKOTA Coupled Model

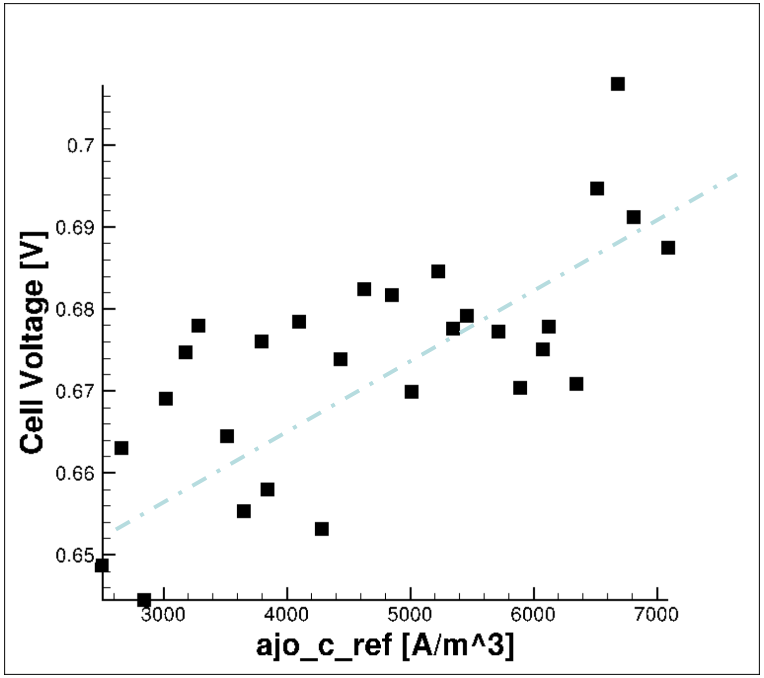
Efficient sensitivity analysis is enabled using the PEMFC/DAKOTA coupled model.

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.

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

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



Thanks to

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

– Program Managers: Jason Marcinkoski
Donna Ho