SAND2011-7309C

Validation of PEMFC Computer Models Using Segmented Current and Temperature Data

ECS Boston 2011

October 9-14, 2011

Brian Carnes* and Ken S. Chen

Sandia National Laboratories

Dusan Spernjak

Los Alamos National Laboratory

Gang Luo

Penn State University

*** bcarnes@sandia.gov**

Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

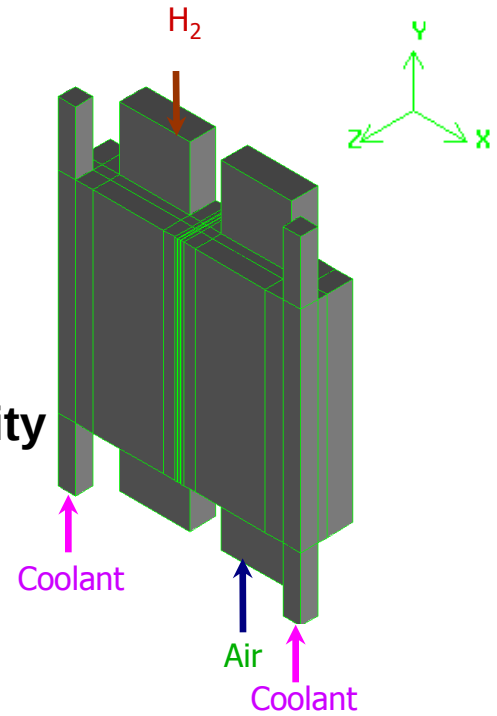
Motivation

- Improve understanding of the limits of the predictive capability of computational fuel cell models
- Demonstrate model validation using high resolution (10x10) segmented current density data
- Utilize segmented temperature data as a boundary condition in model validation
- Include uncertainty in experimental data and model inputs

Sandia National Laboratories

3D Two-Phase PEMFC Model

- Model developed at Penn State University (ECEC group led by C-Y Wang)
- 3D finite volume model implemented in FLUENT
  - Extensive use of user-defined functions (UDFs)
- Multiple coupled physical phenomena
  - Two-phase flow (CL, GDL, channel)
  - Non-isothermal, non-uniform density
  - Electrical/ionic transport
  - Species transport (H2, O2, H20, N2)
  - MPL model for liquid water saturation discontinuity
- Ongoing work
  - Improved GDL/channel interface condition
  - Model validation



Sandia National Laboratories

Experimental Data

Inputs	Outputs
• Current Density (CD) • Stoich (a/c) • Cell Temperature • Back Pressure (a/c) • Relative Humidity (RH) (a/c) • …	• Cell Voltage • Local Current Density • Local Temperature • HFR • Water Balance • …

We are investigating the use of local temperature as a model input (in place of a uniform temperature) for the cathode current collector

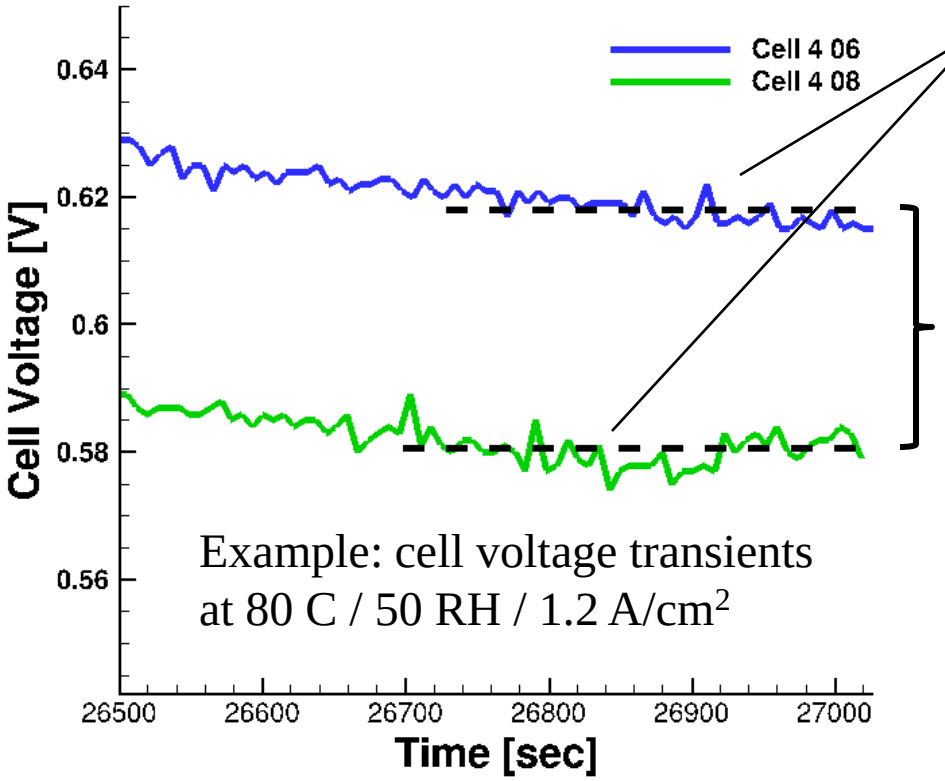
Model Input Parameters

- **The validation experiments were performed at well-defined operating conditions**
  - **Back pressure, stoich, RH for anode/cathode (25, 50, 75, 100%)**
  - **Operating cell temperature (80 and 60 C)**
  - **Current density – 0.1, 0.4, 0.8, 1.0, 1.2 A/cm^2**
- **Other parameters (material properties) came from literature or were measured experimentally**

TABLE I. Model input parameters. (A/C denotes Anode/Cathode)

Parameter	Value	Parameter	Value
Cell temperature [C]	60, 80	A/C back pressure [atm]	1.7/1.7
A/C stoich	1.2/2.0	Cell active area [cm^2]	50
A/C rel. humidity [%]	25-50-75-100	Channel area [mm^2]	1.01
Thermal cond. (plate) [W/m K]	20	Thermal cond. (GDL) [W/m K]	1
Thermal cond. (MPL) [W/m K]	1	Thermal cond. (CL) [W/m K]	1
Thermal cond. (mem) [W/m K]	0.95	Permeability (all) [m^2]	1e-12
Porosity (all)	0.6	Contact angle (all) [deg]	92
Contact resist (GDL-plate) [Ω m^2]	0.1e-6	Contact resist (MPL-CL) [Ω m^2]	0.1e-6

Uncertainty in Experimental Data

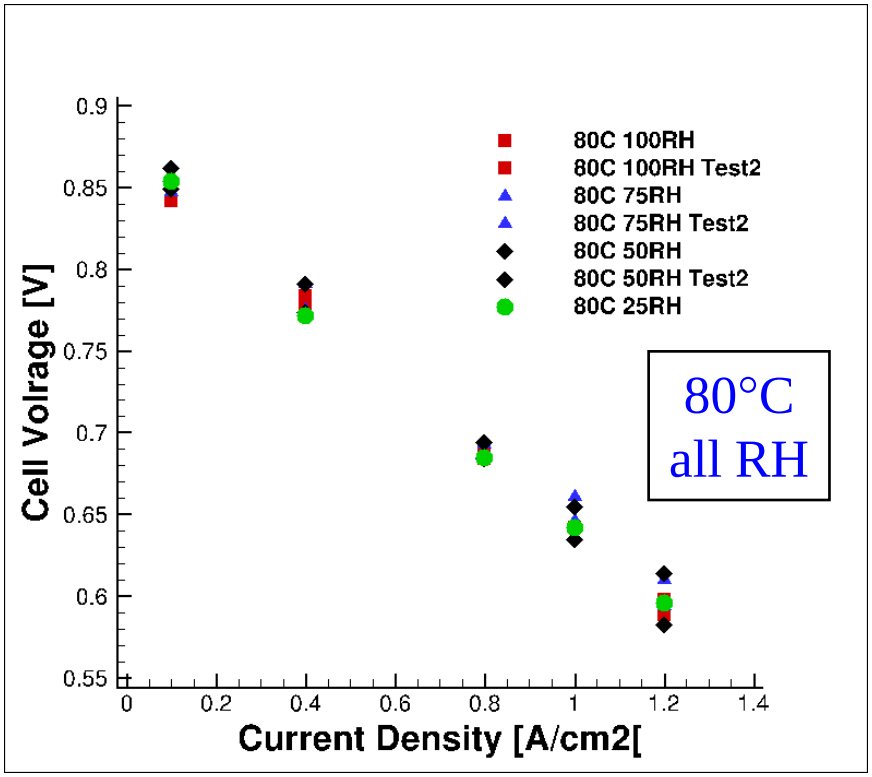


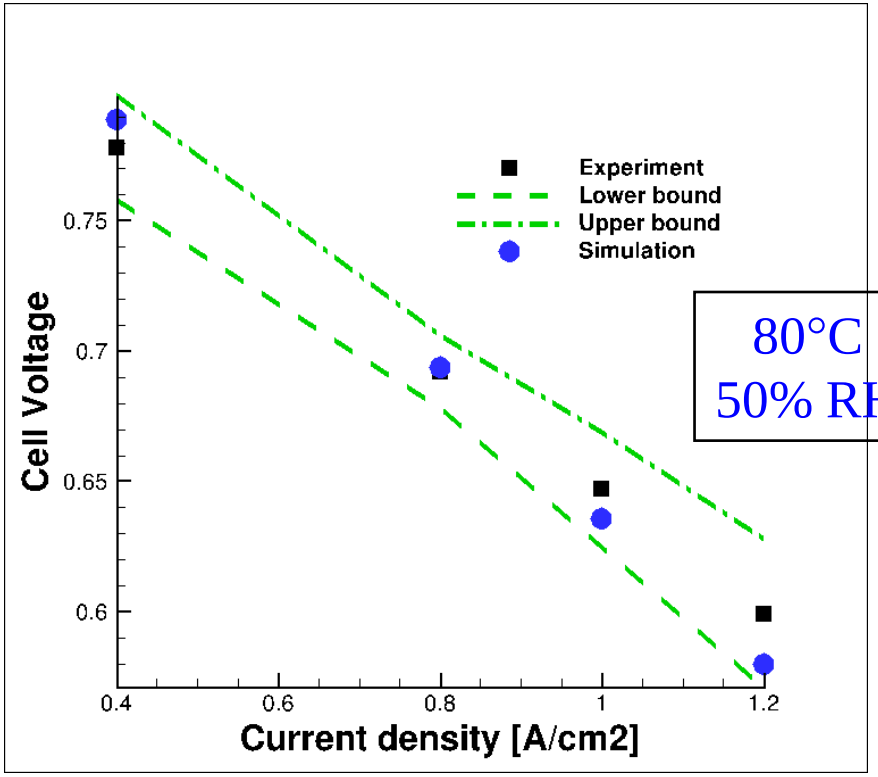
- Uncertainty must be quantified to properly use exp data in model validation
- <u>Random fluctuations</u>
  - Time averaging gives mean & std deviation estimates
  - Use 99% confidence intervals for bounds on uncertainty
- <u>Unit-to-unit variability</u>
  - Often larger than randomness, small sample size
  - Best estimate is interval uncertainty

We generate combined uncertainty bound including both sources of uncertainty

Sandia National Laboratories

Calibration using Cell Voltage (80 C)





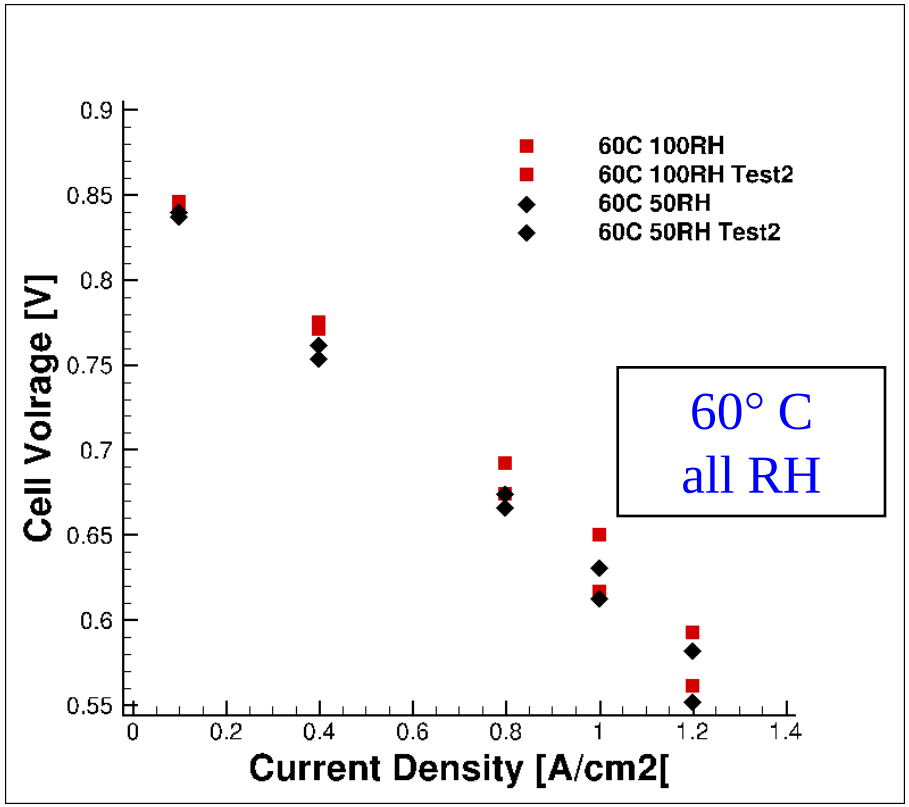
Experimental data from LANL at 80°C (note variability from repeated tests)

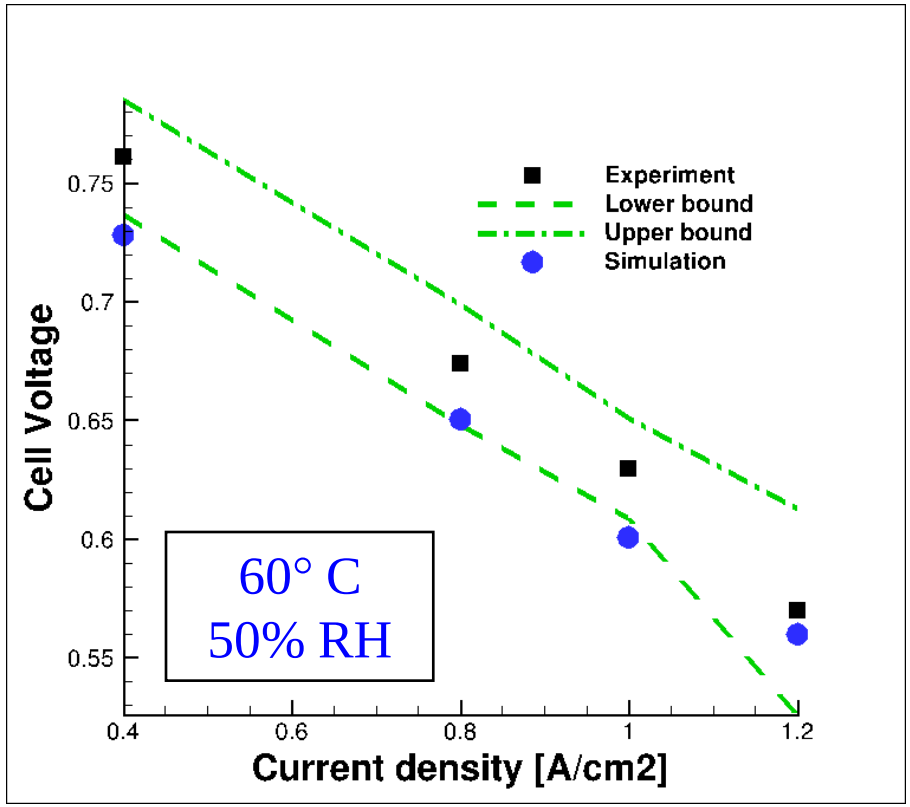
Model calibration at 80° within uncertainty of the experimental data

Key parameter in calibration: cathode exchange current densityc

Sandia National Laboratories

Validation using Cell Voltage (60 C)





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

Model prediction at 60°C within uncertainty of the experimental data.

Uncertainty provides metric for assessing validation

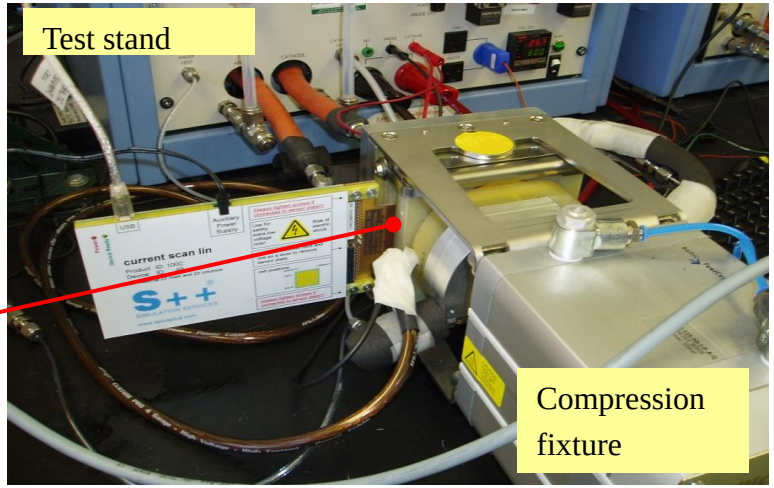
Sandia National Laboratories

Experimental Setup at LANL

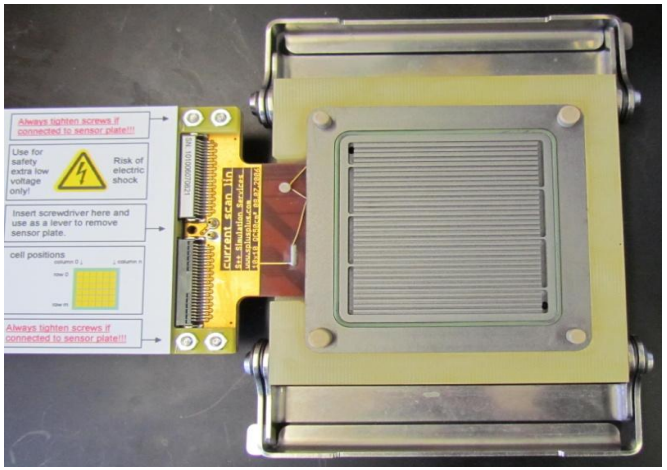
Fuel Cell Assembly 50 cm^2

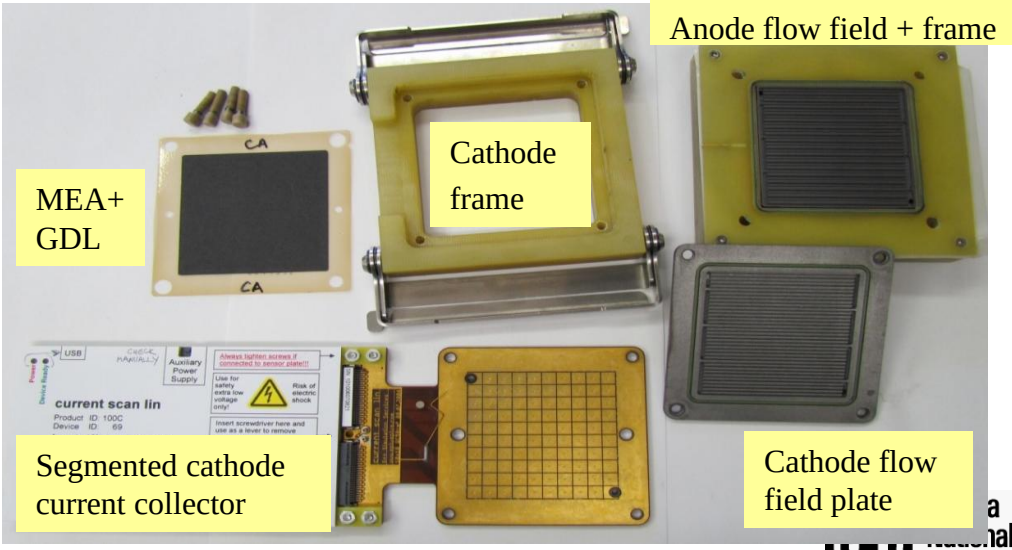
- Current and T Distribution (10 x 10 segments)
- Varying Compression

Assembled fuel cell
w. segmented current collector



Assembled cathode side:
flow field + frame + current collector



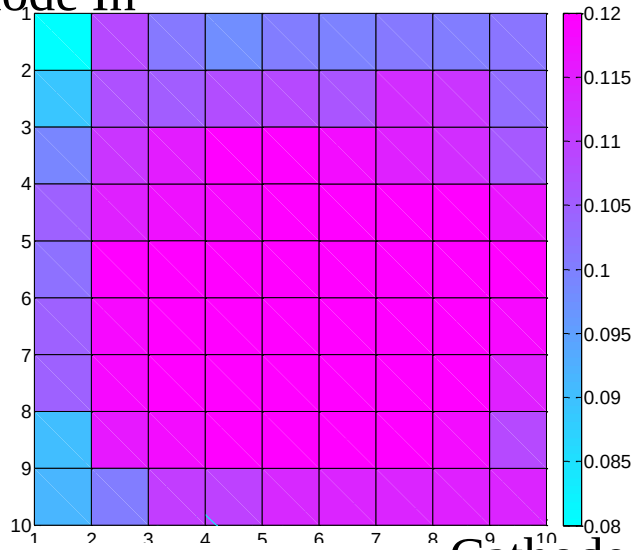


Experimental Measurement of Local CD

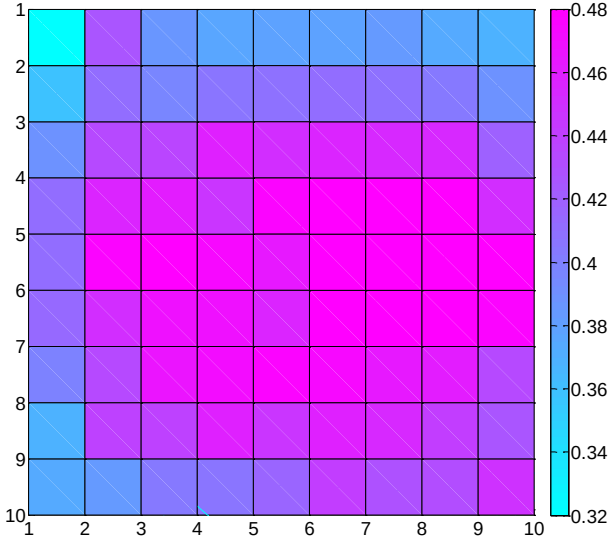
MEA (catalyst coated membrane) = A510.2/M710.18/C510.4 (by W. L. Gore), GDL = SGL24BC (by SGL Carbon)

GDL – 200μm, MPL – 50μm, cathode CL – 20μm, anode CL – 10μm, membrane – 18μm.

Cathode In

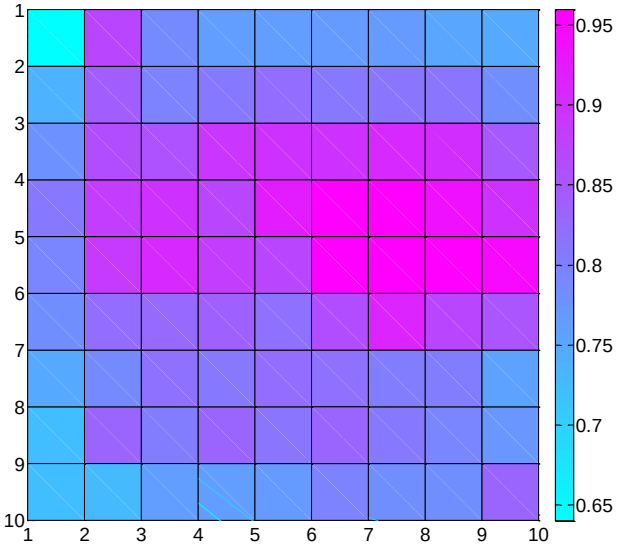


0.1 A/cm^2

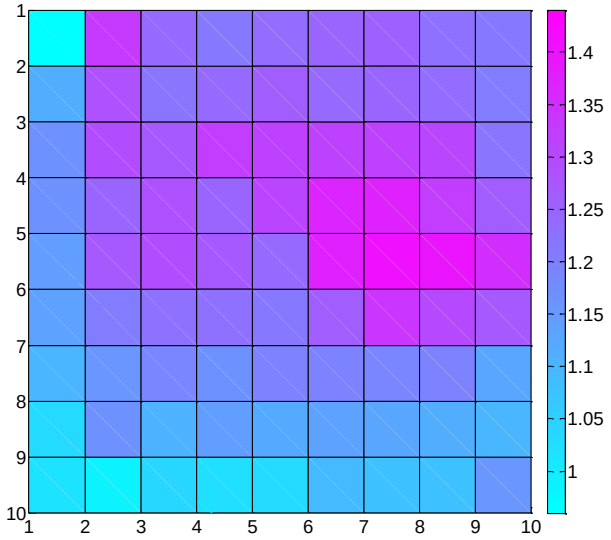


0.4 A/cm^2

Cathode Out



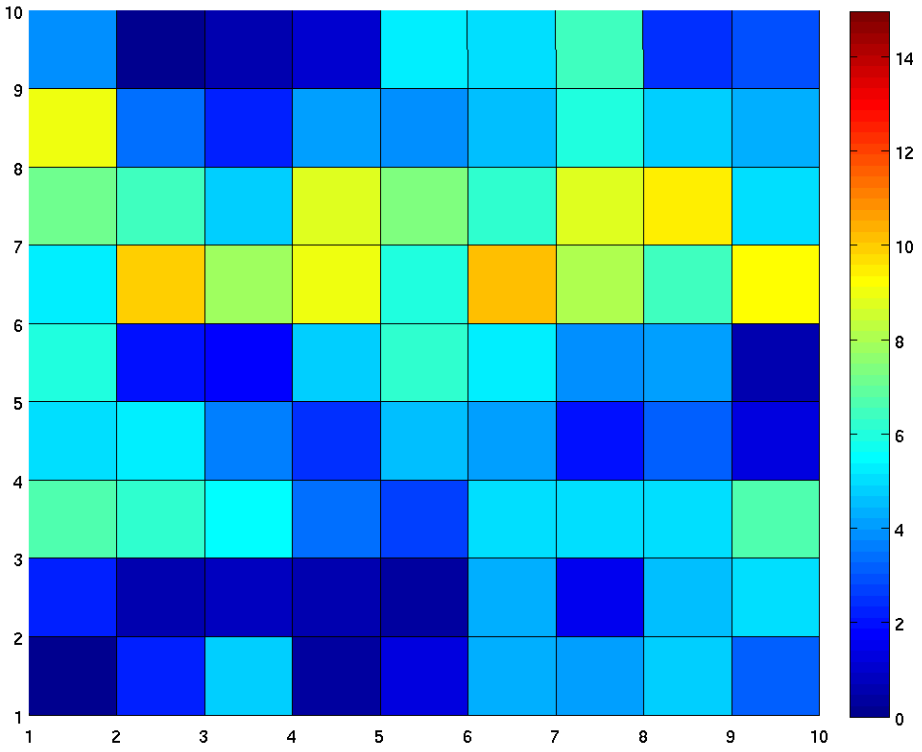
1.0 A/cm^2



1.2 A/cm^2

Uncertainty in Segmented Current Density

- **For multiple measurements of local CD, we can estimate the uncertainty as with voltage**
- **We present the uncertainty as the max distance from the data to the average of the data**
- **For two measurements this is just U = 0.5 * (max(CD) – min(CD))**

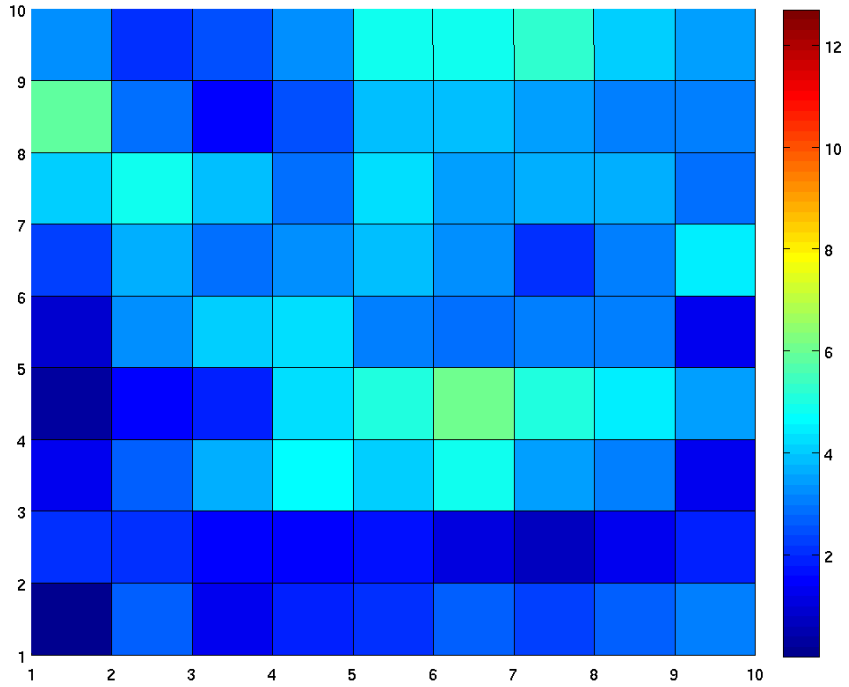


0.1 A/cm^2

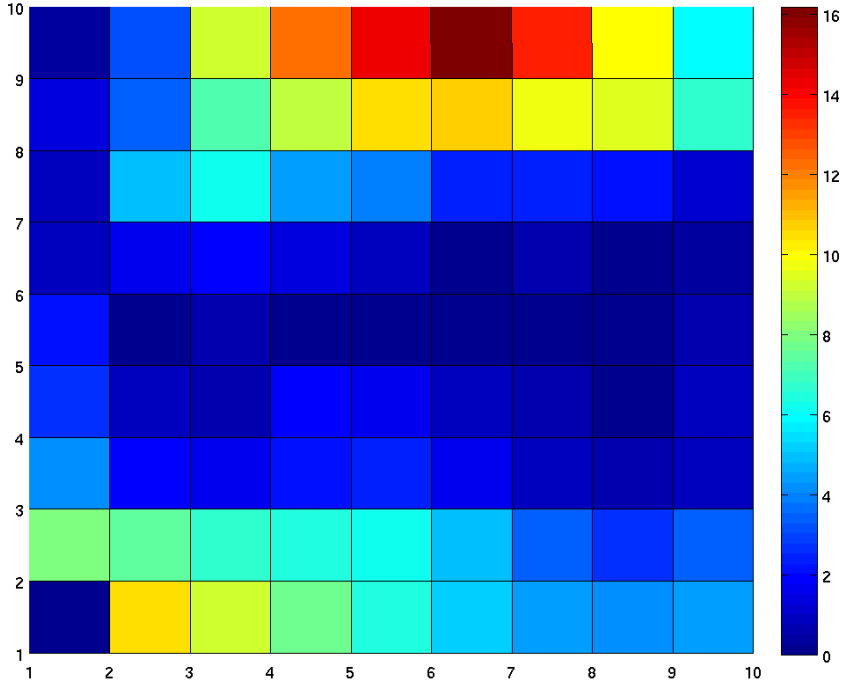
Example of uncertainty in local from two experiments at 80 C / Uncertainty ranges from 0-15%.

Sandia National Laboratories

Uncertainty in Segmented Current Density



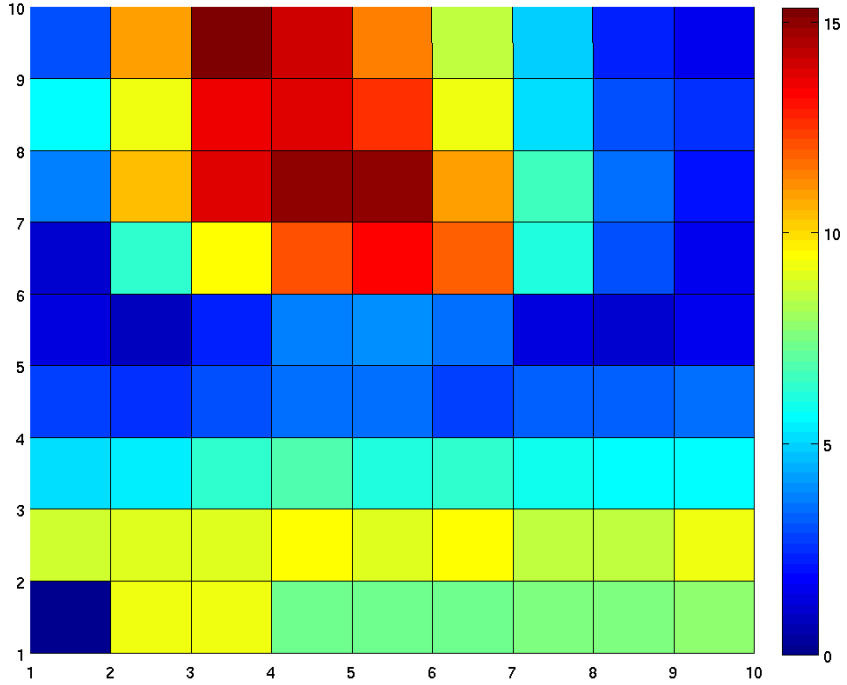
0.4 A/cm^2



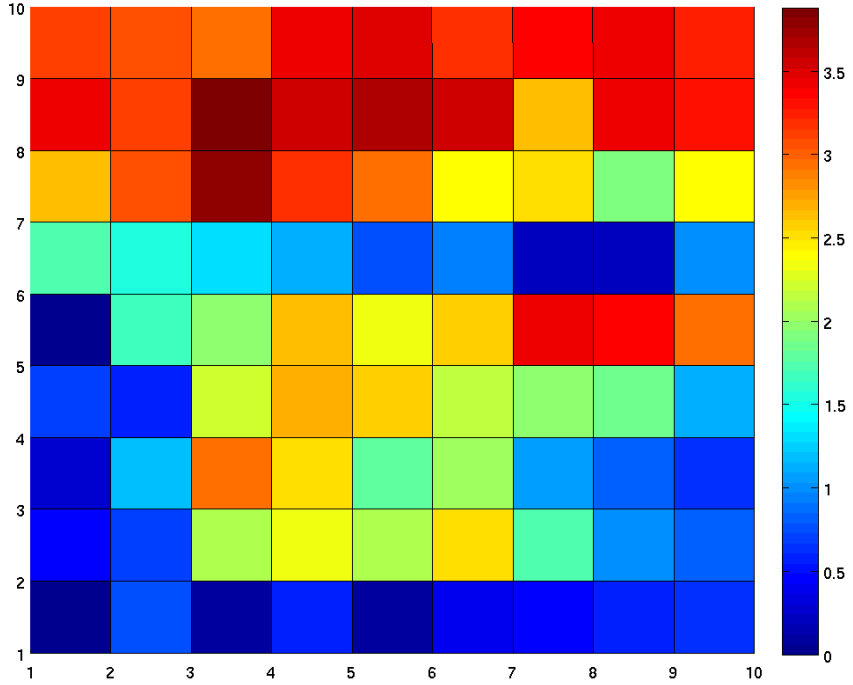
0.8 A/cm^2

Sandia National Laboratories

Uncertainty in Segmented Current Density



1.0 A/cm^2

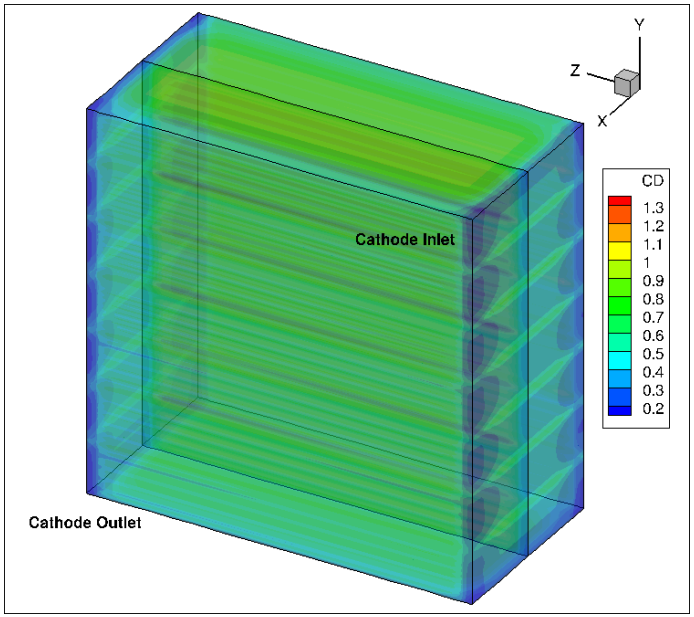


1.2 A/cm^2

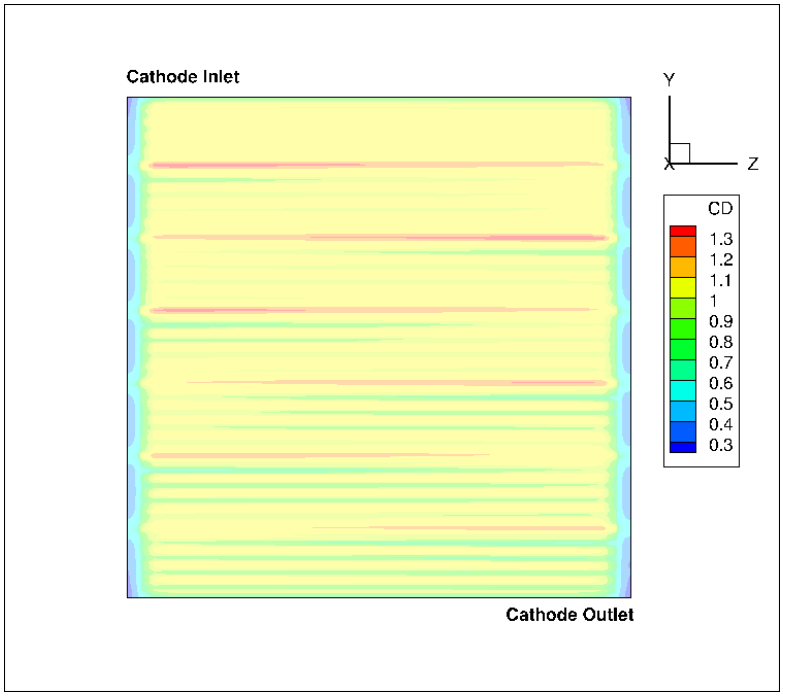
Sandia National Laboratories

Postprocessing Segmented Current Density

- **We compute local current density (CD) throughout the membrane.**
- **Along the center of the membrane, we compute average CD on a 10x10 grid corresponding to the experimental segmented bipolar plate**



Current density in membrane



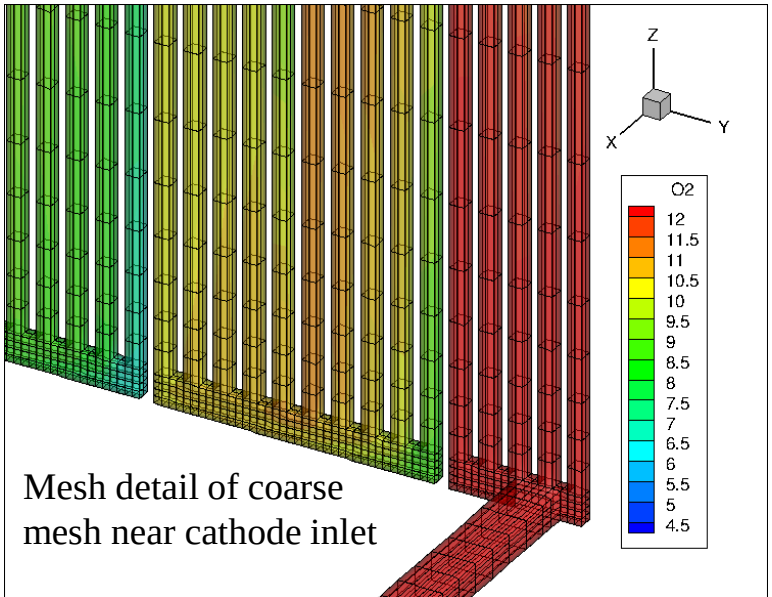
Current density at membrane center

Sandia National Laboratories

Grid Convergence Study

- **Several types of grids have been used: uniform, graded**
- **We need to estimate numerical error (uncertainty) in solution outputs as part of model validation**

	Cells	CPU	Channel	Mem	CCL	GDL+MPL
Coarse	230K	1	2x2	8	10	12
Medium	610K	4	3x3	12	15	18
Fine	2.21M	16	5x5	18	22	28



Mesh detail of coarse mesh near cathode inlet

Inlet	-2.9	-2.9	-3.0	-3.0	-3.1	-3.1	-3.2	-3.3	-4.1
-3.4	-1.9	-2.3	-2.7	-3.2	-3.6	-4.1	-4.7	-5.2	-5.7
-7.6	-6.2	-5.5	-5.0	-4.5	-4.2	-4.2	-4.2	-4.3	-5.0
-3.5	-0.5	0.7	1.8	2.7	3.3	3.7	4.0	4.2	2.7
2.5	5.0	4.8	4.3	3.6	2.7	1.4	-0.2	-2.2	-4.2
-5.6	-2.9	-1.1	0.4	1.5	2.1	2.5	2.7	2.7	1.0
-2.0	1.0	1.5	1.9	2.2	2.3	2.4	2.4	2.3	0.7
4.8	7.6	7.5	7.1	6.5	5.8	4.5	2.8	0.8	-1.9
-3.0	-0.2	0.5	1.2	1.8	2.3	2.7	3.0	3.3	1.8
0.1	2.4	2.5	2.7	3.0	3.2	3.4	3.5	3.3	Out

Numerical error in segmented CD between coarse and medium solution less than about 5%

Sandia National Laboratories

Segmented Current Validation 0.4 A/cm^2

Experimental data (time avgd)

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

Simulation

0.33	0.34	0.34	0.33	0.33	0.33	0.33	0.33	0.33	0.29
0.37	0.39	0.39	0.39	0.39	0.39	0.39	0.39	0.39	0.35
0.39	0.42	0.42	0.42	0.42	0.42	0.42	0.43	0.44	0.39
0.44	0.47	0.46	0.46	0.45	0.45	0.45	0.45	0.45	0.39
0.42	0.45	0.45	0.45	0.45	0.45	0.46	0.46	0.46	0.41
0.42	0.44	0.44	0.44	0.44	0.44	0.44	0.45	0.45	0.40
0.41	0.43	0.43	0.42	0.42	0.42	0.41	0.41	0.41	0.37
0.36	0.38	0.38	0.39	0.39	0.40	0.40	0.40	0.41	0.37
0.34	0.36	0.36	0.37	0.37	0.38	0.38	0.38	0.39	0.35
0.28	0.30	0.31	0.32	0.33	0.34	0.35	0.35	0.36	0.32

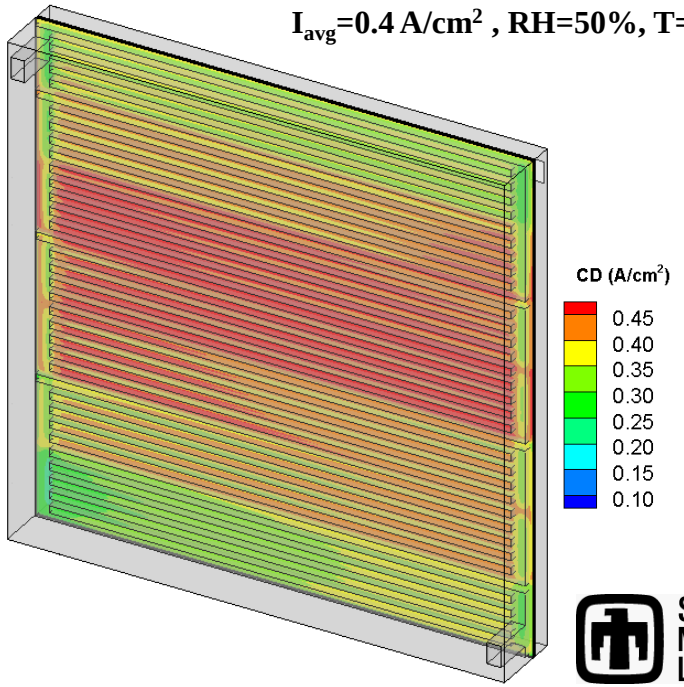
Relative difference between experiments and simulation

0.0%	19.7%	12.4%	11.3%	12.5%	13.5%	14.7%	13.0%	11.7%	22.7%
-4.2%	5.0%	1.7%	5.1%	5.5%	5.9%	5.4%	3.5%	-1.1%	10.8%
-0.4%	4.0%	4.7%	9.2%	7.5%	7.5%	6.2%	5.2%	-4.4%	6.3%
-7.8%	-3.0%	-0.6%	-2.6%	4.7%	10.0%	10.9%	6.8%	1.4%	13.6%
-3.2%	5.7%	7.4%	4.9%	2.3%	10.2%	13.4%	13.3%	6.9%	13.6%
-1.6%	1.9%	5.6%	5.7%	2.9%	9.4%	13.4%	9.8%	6.0%	17.5%
-3.4%	0.5%	8.3%	10.4%	11.8%	12.1%	11.0%	11.3%	6.6%	19.1%
1.5%	13.4%	12.5%	15.6%	12.4%	14.0%	11.9%	8.6%	4.2%	15.0%
9.3%	7.3%	10.0%	9.5%	9.9%	14.1%	10.8%	10.6%	13.7%	12.5%
19.4%	17.2%	0.2%	-15.4%	12.0%	6.3%	6.1%	7.9%	-16.4%	0.0%

$$\text{RMS difference} = \sqrt{\frac{\sum_{i=1}^{100}\left(\frac{I_{Exp}^{i} - I_{Sim}^{i}}{I_{Exp}^{i}}\right)^2}{100}}$$ **=10%**

Predicted membrane current density distribution

I_{avg}=0.4 A/cm^2 , RH=50%, T=80C



Sandia National Laboratories

Segmented Current Validation 1.0A/cm^2

Experimental data (time avgd)

0.00	1.10	1.01	1.01	1.02	1.02	1.02	1.00	0.99	0.98
0.90	1.03	0.97	0.97	0.99	0.97	0.99	0.98	0.96	0.98
0.97	1.06	1.02	1.05	1.06	1.06	1.07	1.07	1.02	1.02
0.99	1.05	1.05	1.01	1.06	1.12	1.13	1.08	1.05	1.09
0.97	1.08	1.09	1.07	1.05	1.16	1.16	1.14	1.12	1.14
0.99	1.07	1.09	1.09	1.06	1.12	1.16	1.12	1.11	1.15
0.98	1.05	1.09	1.06	1.09	1.08	1.06	1.06	1.00	1.07
0.93	1.05	1.01	1.05	1.04	1.05	1.02	1.00	0.99	1.06
0.91	0.90	0.94	0.95	0.96	1.00	0.98	0.98	1.05	0.96
0.84	0.88	0.76	0.67	0.88	0.86	0.88	0.91	0.75	0.00

Simulation

1.05	1.15	1.13	1.12	1.11	1.11	1.10	1.09	1.09	0.94
1.04	1.12	1.12	1.12	1.13	1.13	1.14	1.15	1.16	1.03
1.04	1.11	1.11	1.12	1.12	1.12	1.13	1.14	1.16	1.03
1.04	1.10	1.09	1.07	1.06	1.05	1.04	1.03	1.02	0.93
0.94	1.00	1.00	1.00	1.01	1.01	1.02	1.03	1.05	0.99
0.97	1.00	0.99	0.99	0.99	0.99	0.99	0.99	1.00	0.93
0.96	1.00	0.97	0.96	0.94	0.93	0.92	0.92	0.91	0.85
0.83	0.87	0.88	0.90	0.91	0.92	0.93	0.94	0.95	0.88
0.82	0.86	0.86	0.87	0.87	0.88	0.89	0.90	0.90	0.82
0.72	0.77	0.78	0.79	0.80	0.81	0.82	0.83	0.83	0.77

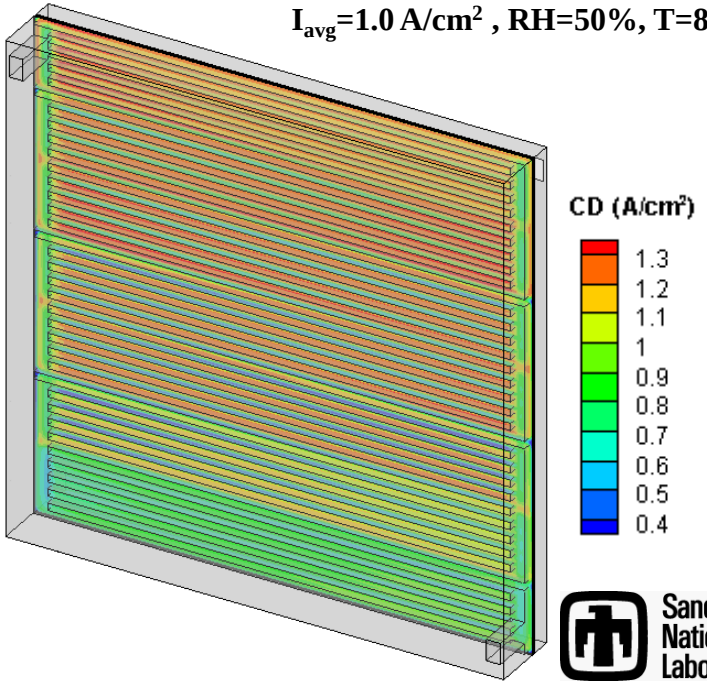
Relative difference between experiments and simulation

0.0%	-4.5%	-12.6%	-11.5%	-9.5%	-8.2%	-7.8%	-9.4%	-9.7%	3.7%
-16.2%	-9.3%	-16.2%	-15.7%	-13.8%	-16.8%	-14.7%	-16.5%	-20.7%	-5.7%
-7.9%	-5.3%	-9.4%	-6.1%	-6.1%	-5.8%	-5.8%	-6.2%	-13.6%	-0.4%
-4.9%	-5.2%	-3.4%	-5.8%	0.2%	6.2%	7.9%	4.6%	3.0%	14.9%
3.2%	6.8%	8.3%	7.0%	4.2%	12.4%	11.7%	9.1%	6.1%	13.6%
2.3%	6.7%	9.1%	9.3%	7.0%	11.3%	14.4%	11.1%	9.4%	18.9%
2.1%	5.1%	10.6%	10.1%	13.7%	13.3%	12.4%	13.3%	9.1%	20.5%
10.5%	16.5%	12.8%	14.9%	12.5%	12.3%	8.6%	6.1%	3.6%	16.6%
9.2%	5.0%	7.9%	8.6%	8.9%	12.1%	8.9%	8.3%	13.8%	14.1%
14.1%	11.9%	-2.9%	-17.1%	9.1%	5.8%	6.9%	8.8%	-10.2%	0.0%

$$\text{RMS difference} = \sqrt{\frac{\sum_{i=1}^{100}\left(\frac{I_{Exp}^{i} - I_{Sim}^{i}}{I_{Exp}^{i}}\right)^2}{100}} = 11\%$$

Predicted membrane current density distribution

I_{avg}=1.0 A/cm^2 , RH=50%, T=80C



Sandia National Laboratories

Segmented Current Validation 1.2A/cm^2

Experimental data (time avgd)

0.00	1.37	1.26	1.24	1.25	1.26	1.26	1.23	1.21	1.20
1.12	1.28	1.18	1.20	1.22	1.20	1.22	1.23	1.20	1.22
1.17	1.27	1.21	1.26	1.28	1.27	1.30	1.30	1.24	1.25
1.18	1.24	1.23	1.18	1.25	1.32	1.33	1.28	1.24	1.31
1.14	1.22	1.23	1.20	1.18	1.31	1.31	1.31	1.28	1.34
1.17	1.24	1.25	1.25	1.22	1.28	1.33	1.30	1.29	1.36
1.15	1.22	1.28	1.24	1.27	1.25	1.24	1.23	1.18	1.28
1.10	1.23	1.19	1.23	1.20	1.21	1.18	1.19	1.16	1.26
1.08	1.05	1.10	1.10	1.11	1.16	1.14	1.15	1.23	1.14
1.01	1.04	0.89	0.79	1.03	1.00	1.03	1.07	0.88	0.00

Simulation

1.31	1.44	1.42	1.40	1.38	1.36	1.34	1.33	1.31	1.16
1.25	1.35	1.34	1.35	1.35	1.35	1.36	1.37	1.38	1.26
1.25	1.32	1.32	1.32	1.33	1.34	1.35	1.35	1.36	1.23
1.25	1.33	1.30	1.28	1.27	1.25	1.24	1.23	1.22	1.13
1.14	1.19	1.18	1.18	1.20	1.21	1.22	1.24	1.26	1.21
1.18	1.20	1.19	1.19	1.18	1.18	1.19	1.19	1.20	1.13
1.15	1.20	1.18	1.15	1.13	1.12	1.11	1.10	1.09	1.04
1.00	1.04	1.05	1.06	1.07	1.08	1.10	1.12	1.14	1.07
1.01	1.03	1.04	1.04	1.04	1.05	1.06	1.07	1.07	0.99
0.91	0.97	0.96	0.97	0.97	0.97	0.98	0.98	0.98	0.92

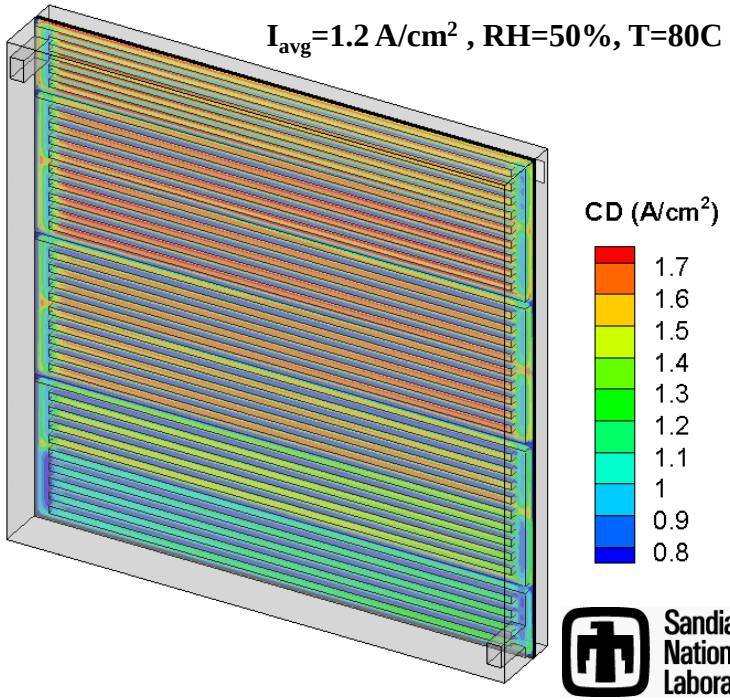
Relative difference between experiments and simulation

0.0%	-4.4%	-12.5%	-12.4%	-9.9%	-7.9%	-6.6%	-7.8%	-8.1%	3.7%
-12.2%	-5.1%	-13.8%	-12.1%	-10.4%	-13.1%	-11.1%	-11.4%	-14.9%	-3.2%
-7.2%	-4.1%	-9.5%	-4.9%	-4.5%	-5.1%	-3.6%	-4.4%	-9.6%	1.3%
-5.3%	-7.1%	-6.1%	-8.2%	-1.7%	4.9%	6.8%	3.7%	1.8%	13.8%
0.4%	2.7%	4.4%	1.3%	-1.0%	7.4%	6.8%	5.0%	0.8%	9.4%
-0.6%	2.8%	4.9%	4.8%	3.2%	7.4%	10.6%	8.4%	6.6%	16.5%
-0.1%	1.6%	7.8%	6.8%	10.5%	10.8%	10.6%	11.1%	7.9%	18.5%
9.2%	15.9%	12.1%	13.8%	11.3%	10.7%	6.8%	5.8%	2.4%	14.5%
6.6%	1.5%	5.4%	5.3%	5.6%	9.3%	7.4%	7.0%	12.9%	13.4%
9.8%	7.3%	-8.3%	-22.7%	5.7%	2.7%	5.3%	8.2%	-11.8%	0.0%

$$\text{RMS difference} = \sqrt{\frac{\sum_{i=1}^{100}\left(\frac{I_{Exp}^{i} - I_{Sim}^{i}}{I_{Exp}^{i}}\right)^2}{100}} = 9\%$$

Predicted membrane current density distribution

I_{avg}=1.2 A/cm^2 , RH=50%, T=80C

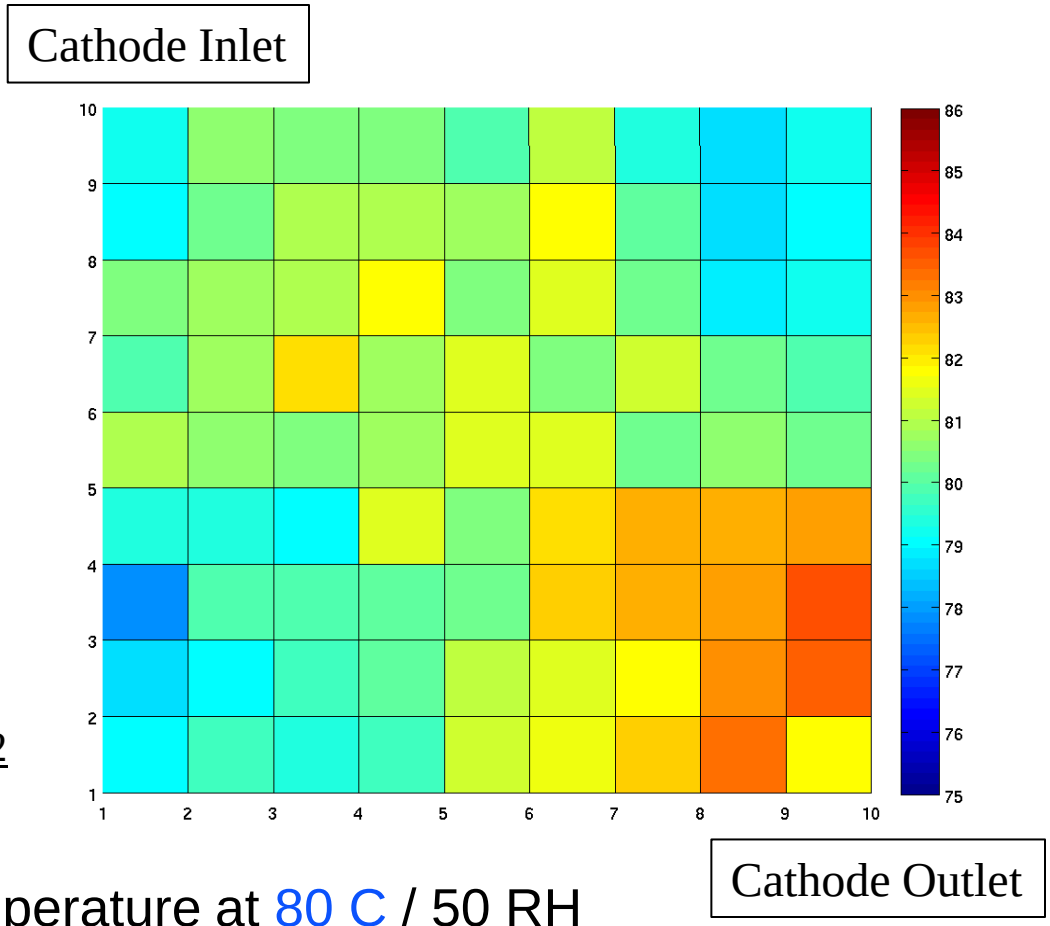


Sandia National Laboratories

Local Temperature Data

- **Temperature can be measured using the segmented current collector**
- **Measurements are taken at OCV immediately after a fixed current step**
- **Averaging of temperature over one minute (versus 6 minutes for current)**

$0.1\ A/cm^2$



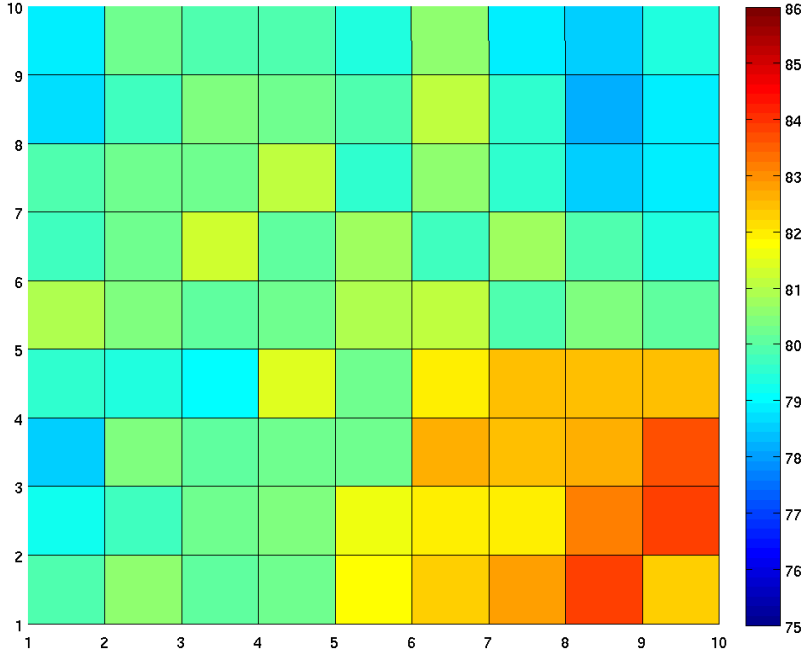
Example of measured local temperature at 80 C / 50 RH

Local temperature can range from 75-86 C.

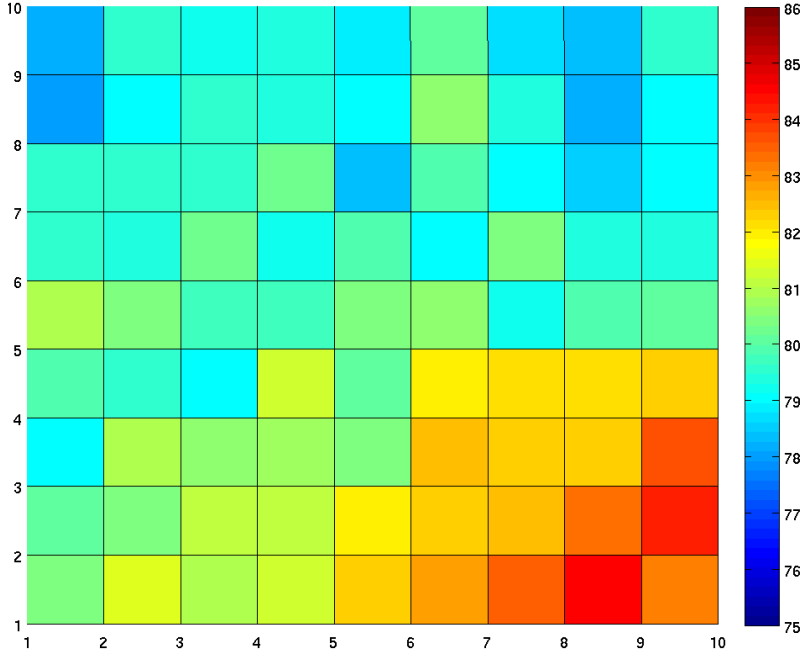
Sandia National Laboratories

Local Temperature Data

Temp measured at 80 C / 50 RH



0.4 A/cm^2

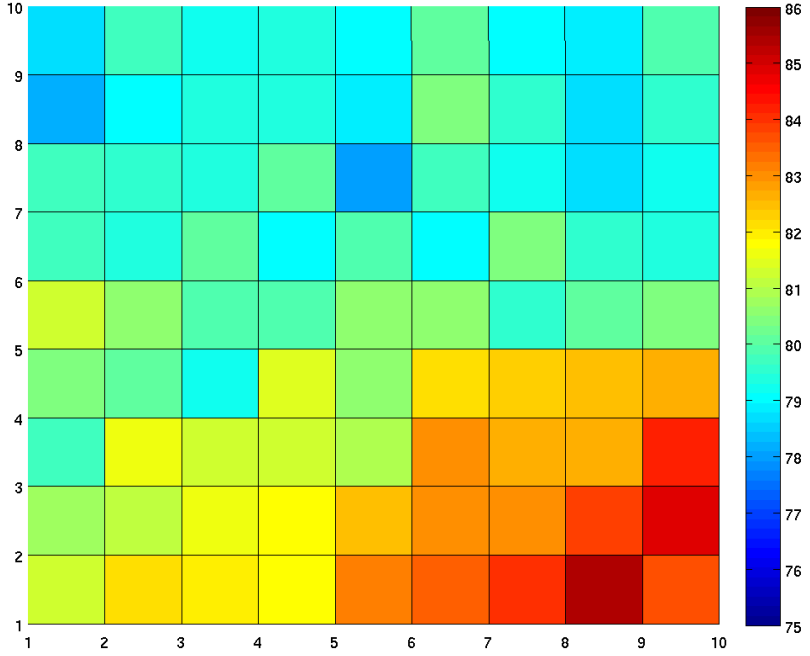


0.8 A/cm^2

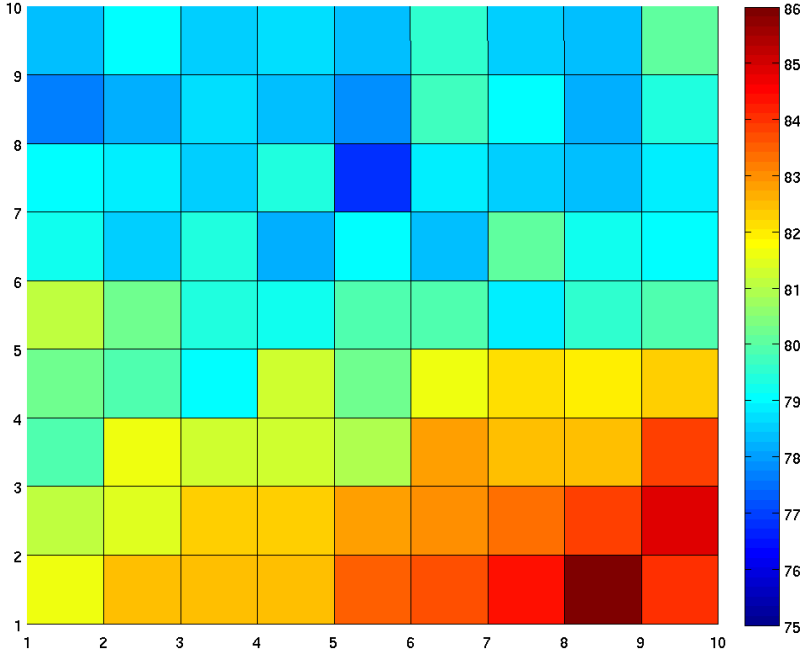
Sandia National Laboratories

Local Temperature Data

Temp measured at 80 C / 50 RH



1.0 A/cm^2



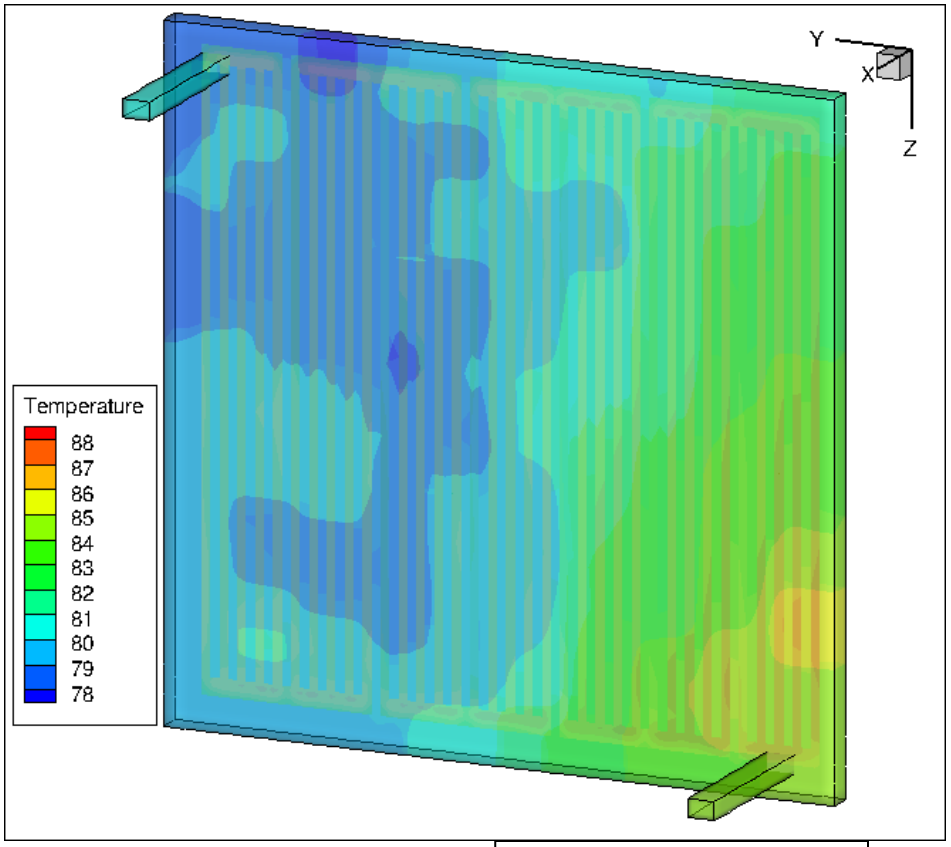
1.2 A/cm^2

Sandia National Laboratories

Local Temperature as Boundary Condition

- **We are investigating using the local temp on the cathode collector as an alternative for the uniform temp BC**
- **A user subroutine interpolates the 10x10 local temperature onto the cathode wall (collector region)**
- **Anode temperature is assumed uniform using the nominal value**

Cathode Inlet



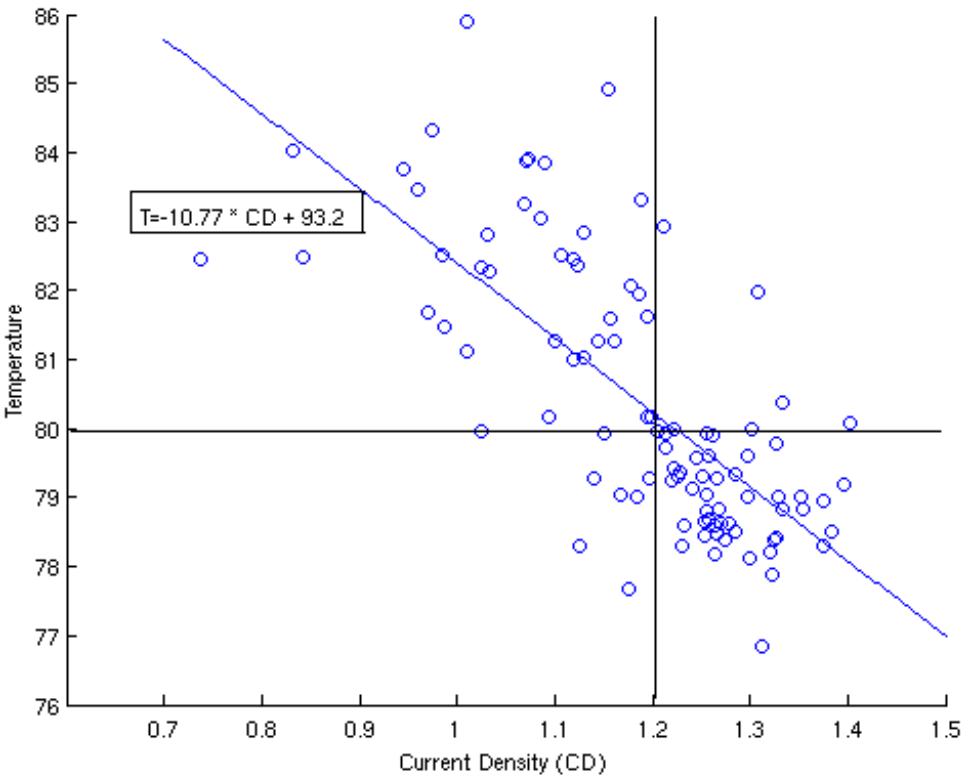
Cathode Outlet

Compute model temp at 80 C / 50 RH / 1.2 CD using the local temperature BC from the exp data.

Sandia National Laboratories

Correlation Between Local CD and Temp

- We estimated the correlation between local CD and T in the data.
- We see an increasing negative correlation between CD and T as the CD increases.
  - Increase of 1º C results in decrease of about 100 mA/cm^2
- This suggests that at higher current densities, local increases in T should result in local decreases in CD.

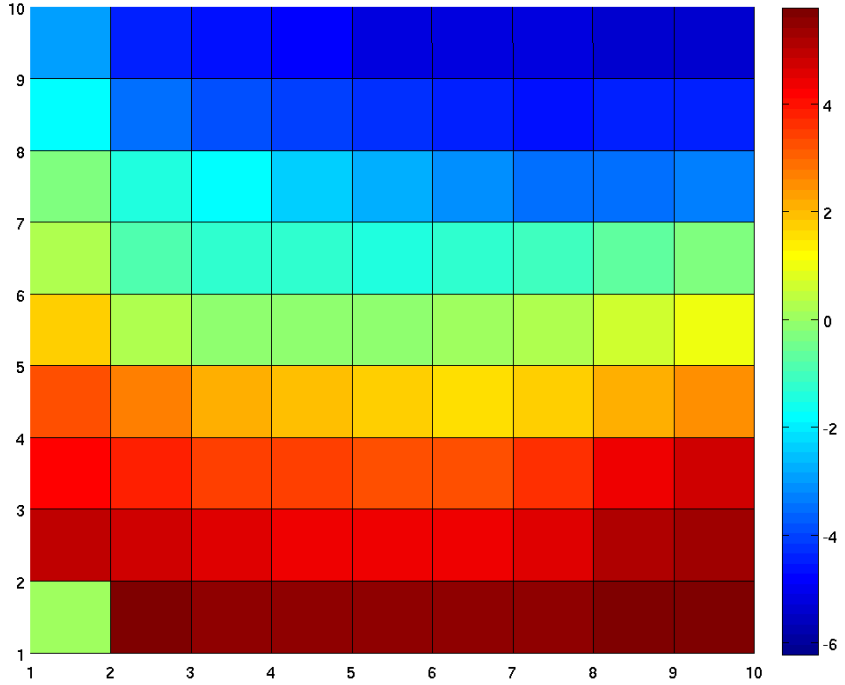


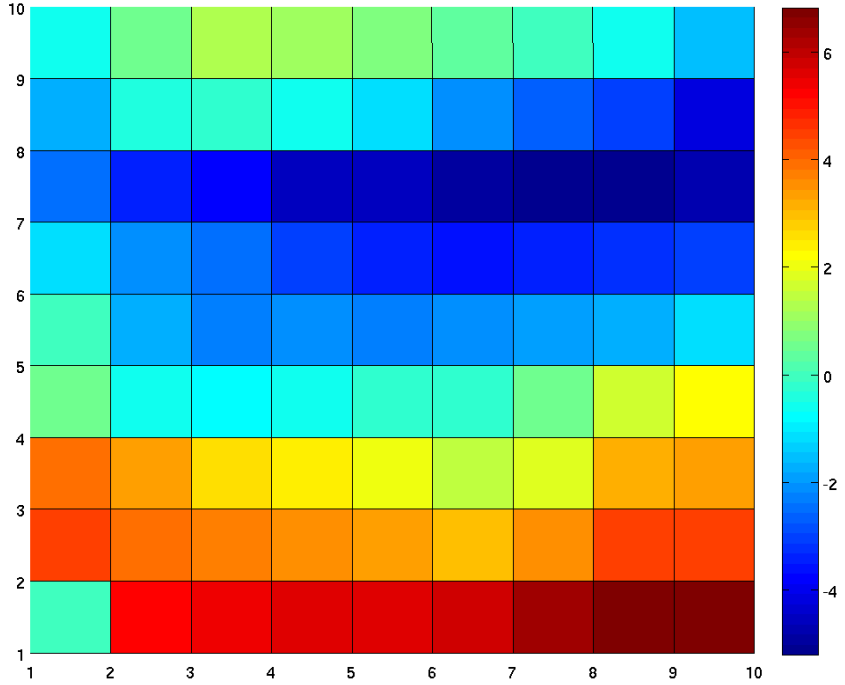
Scatter plot of CD vs. T at 80 C / 50 RH / 1.2 CD along with linear regression fit to data. Correlation coeff is -0.71.

Sandia National Laboratories

Effect of Local Temp BC on Local CD

Percent change in local CD from uniform temp BC at 80 C / 50 RH





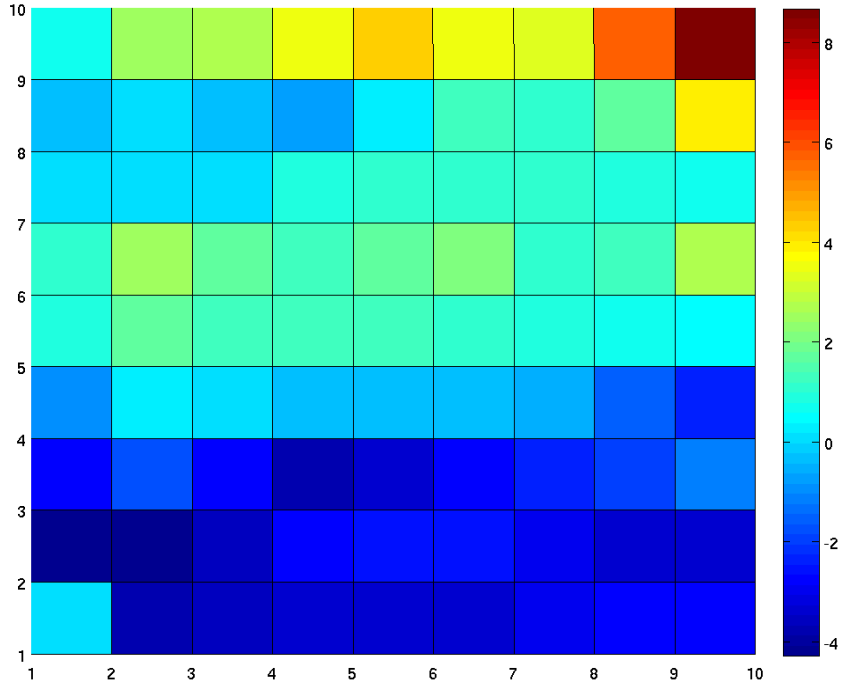
0.1 A/cm^2 0.4 A/cm^2

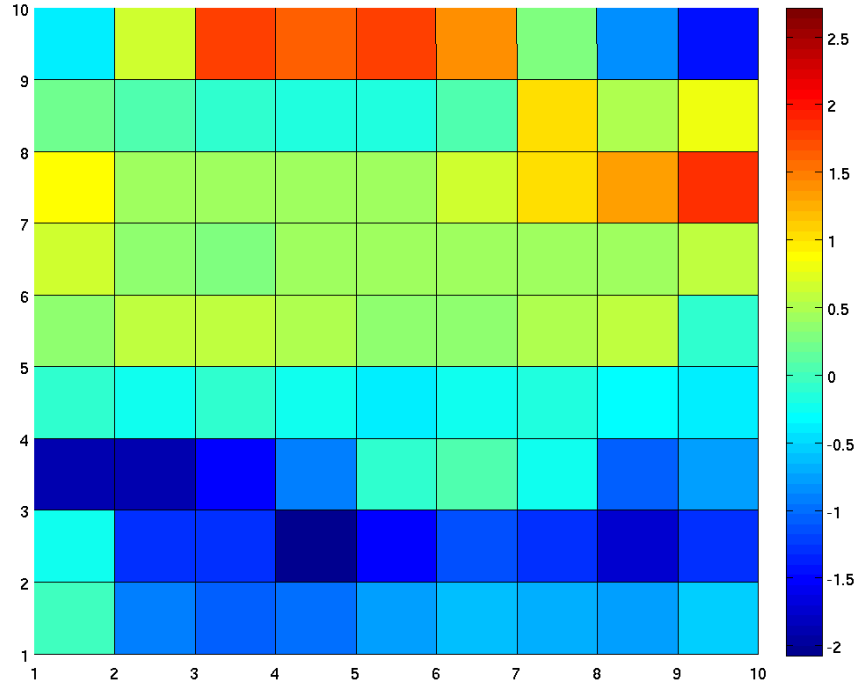
At low CD, increase of CD near outlet

Sandia National Laboratories

Effect of Local Temp BC on Local CD

Percent change in local CD from uniform temp BC at 80 C / 50 RH





0.8 A/cm^2 1.2 A/cm^2

At high CD, increase of CD near inlet

Sandia National Laboratories

Conclusions

- **We have shown adequate model validation for**
  - **Cell voltage**
  - **Local current density**
- **Validation under uncertainty**
  - **Uncertainty provides measure of acceptable agreement with data**
- **Local temperature as boundary condition**
  - **Provides more realistic thermal model**
  - **Local temperature is negatively correlated with local CD**
  - **Also affects local CD, which could improve validation**