SAND2011-5620C

VALIDATION AND UNCERTAINTY QUANTIFICATION OF A TWO-PHASE, MULTIDIMENSIONAL PEMFC COMPUTER MODEL USING HIGH-RESOLUTION SEGMENTED CURRENT COLLECTOR DATA

ASME Fuel Cell 2011

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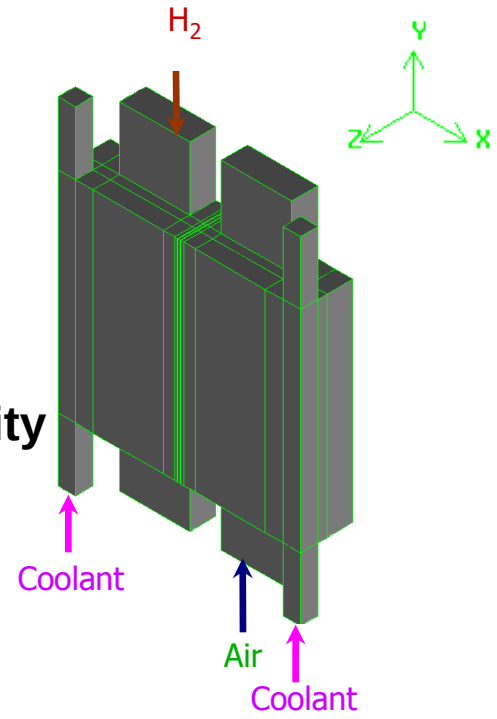
Motivation

- **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**
- **Apply principles from sensitivity analysis and uncertainty quantification to understand**
  - **Effect of parametric uncertainty on model predictions**
  - **Effect on data variability on model validation**

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
  - GDL/channel interface condition
  - Model validation



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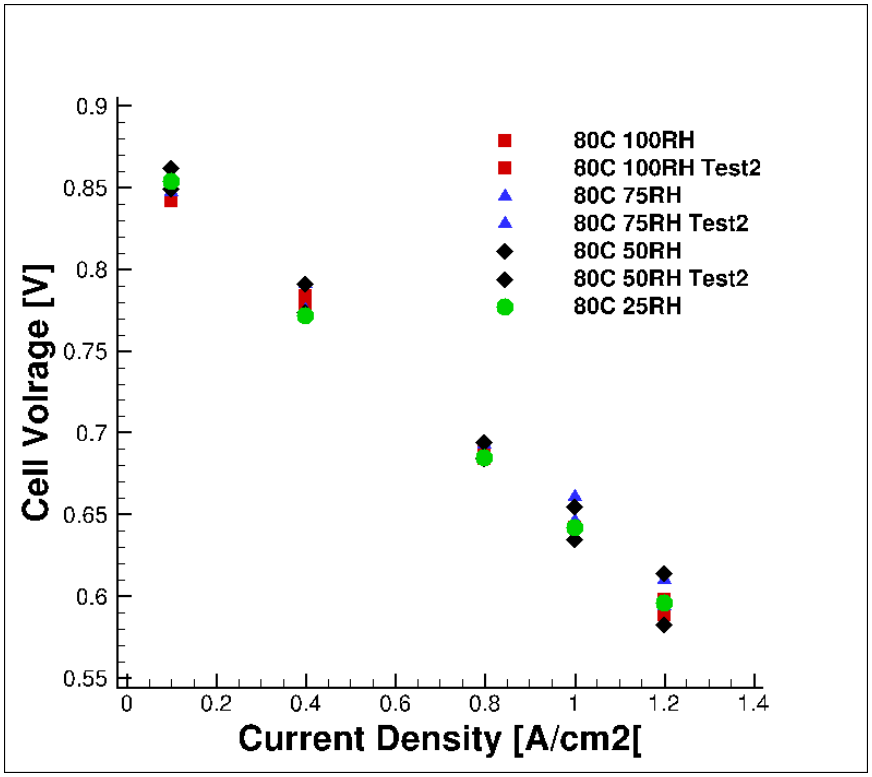
Model Input Parameters

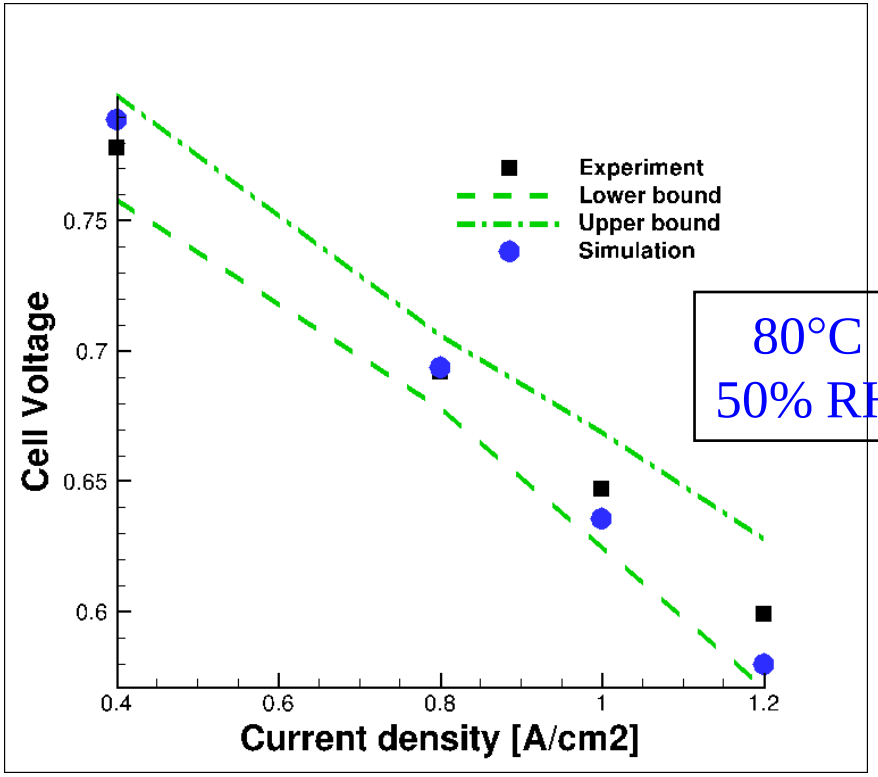
- **The validation experiments were performed at well-defined operating conditions**
  - **Back pressure, stoich, RH for anode/cathode**
  - **Operating cell temperature**
- **Other parameters (material properties) came from literature or were measured experimentally**

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

Parameter	Value	Parameter	Value
Cell temperature [C]	80	A/C back pressure [atm]	1.95/1.95
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) [$\Omega\ m^2$]	0.1e-6	Contact resist (MPL-CL) [$\Omega\ m^2$]	0.1e-6

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 density

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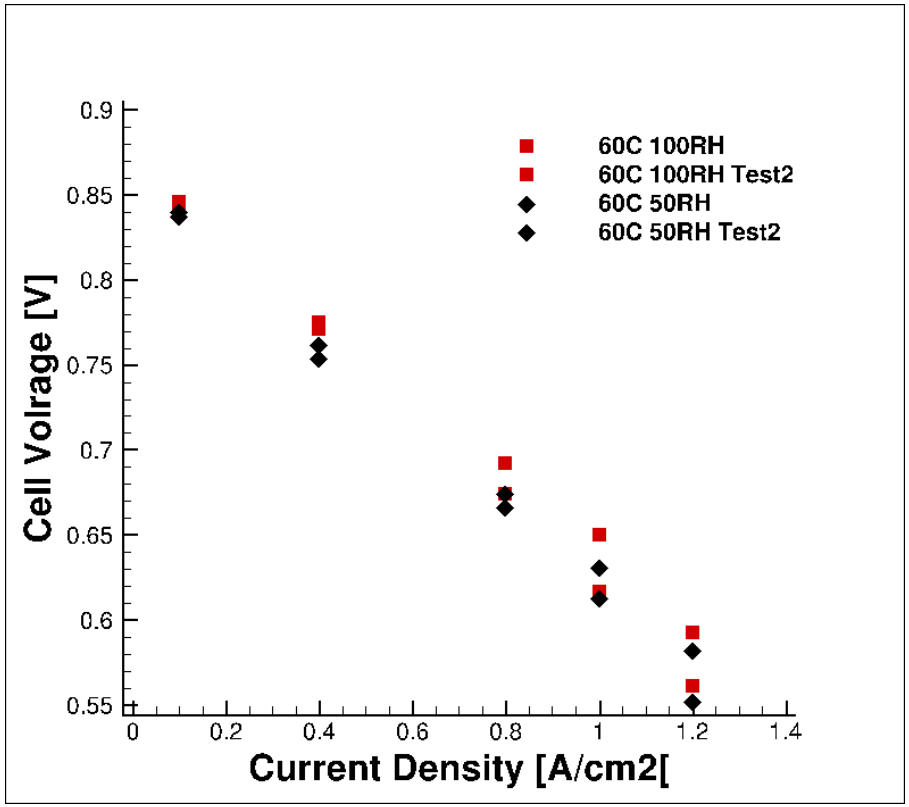
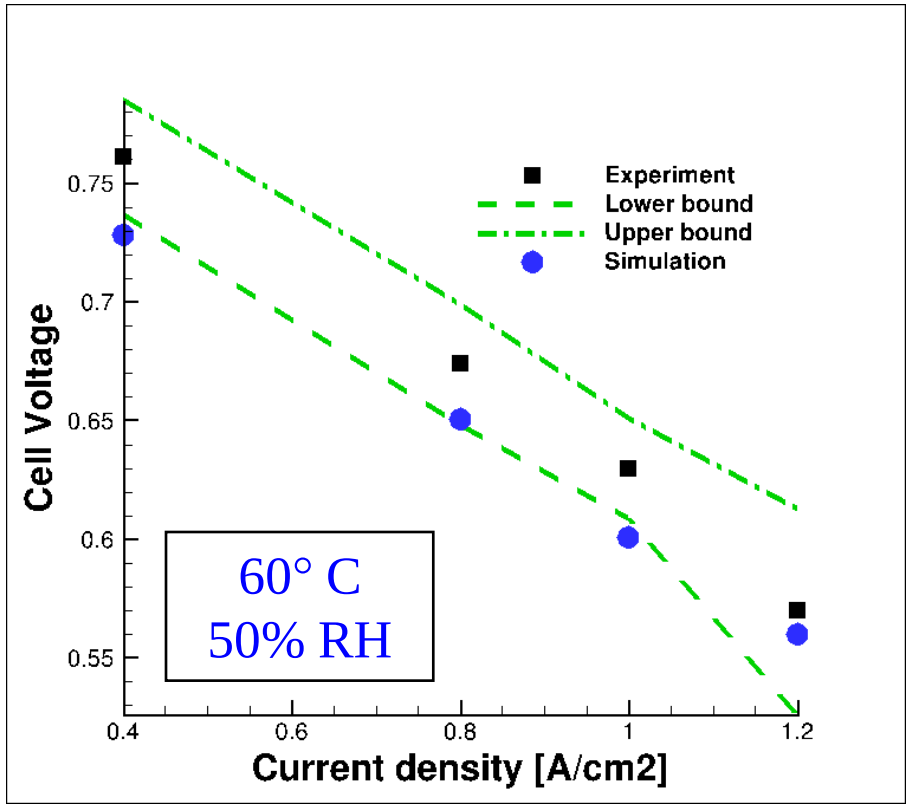
Validation using Cell Voltage (60 C)





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

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

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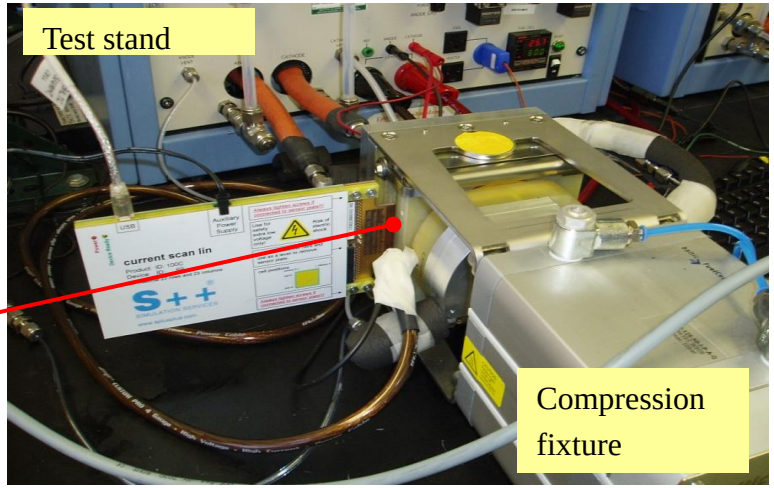
Experimental Setup at LANL

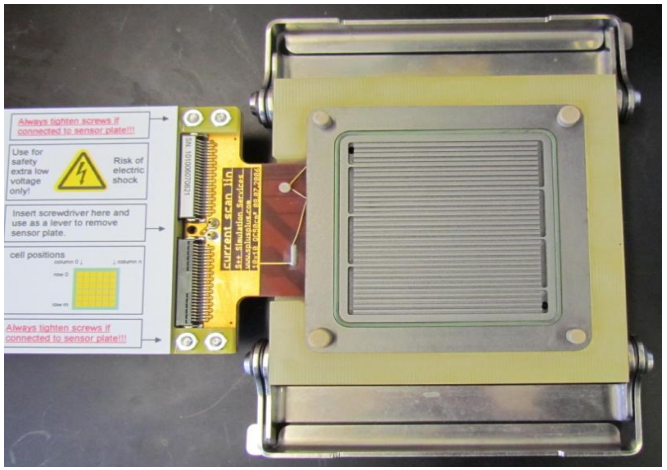
Fuel Cell Assembly 50 cm^2

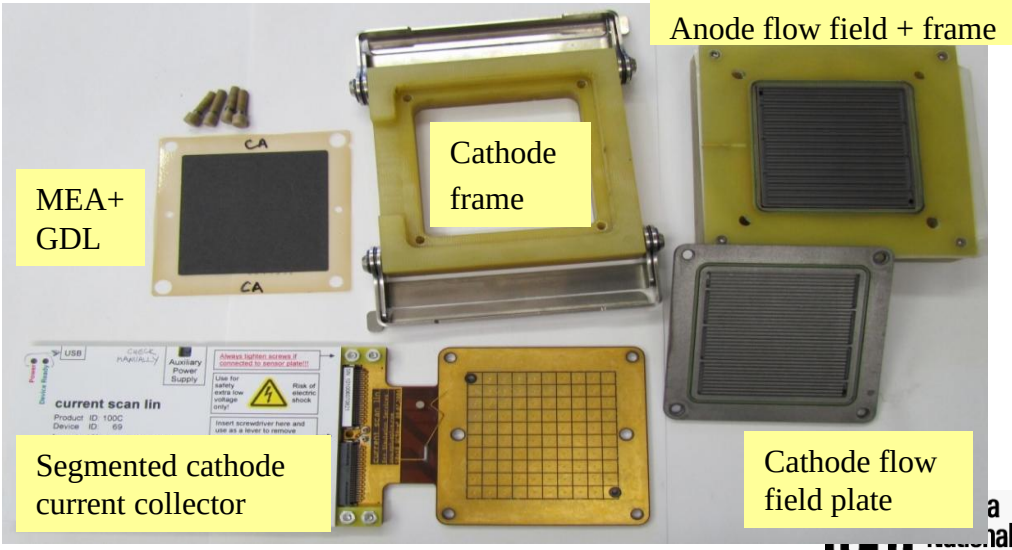
- Current and T Distribution (10 x 10 segments)
- Varying Compression

Assembled fuel cell
w. segmented current collector



Assembled cathode side:
flow field + frame + current collector



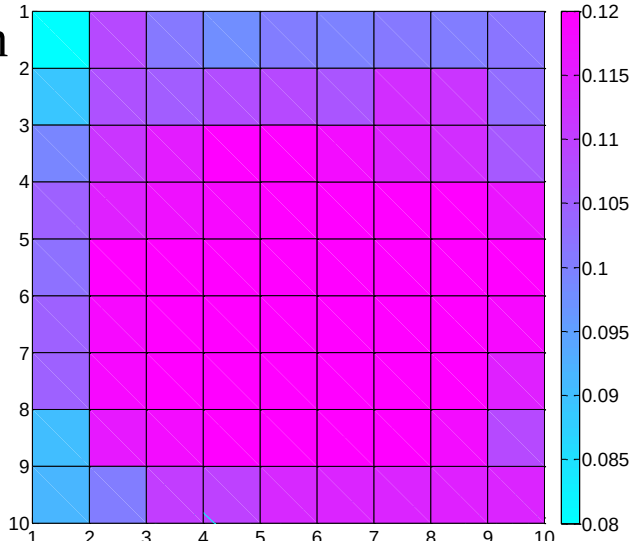


Experimental Measurement of Local CD

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

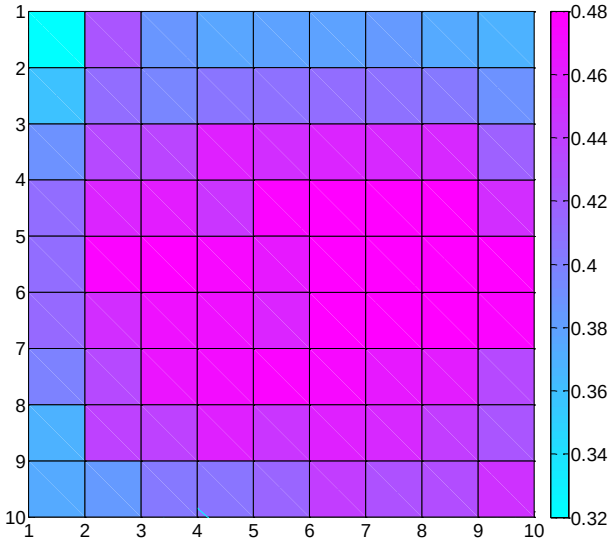
GDL – 200μm, MPL – 50μm, cathode CL – 20μm, anode CL – 10μm, membrane – 18μm.

In

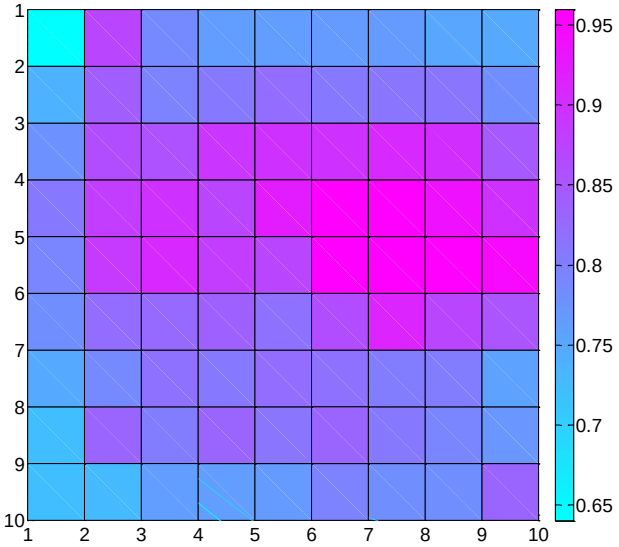


0.1 A/cm^2

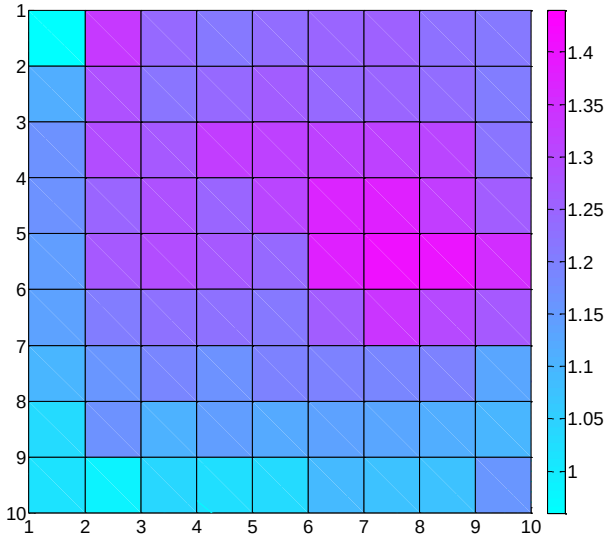
Out



0.4 A/cm^2



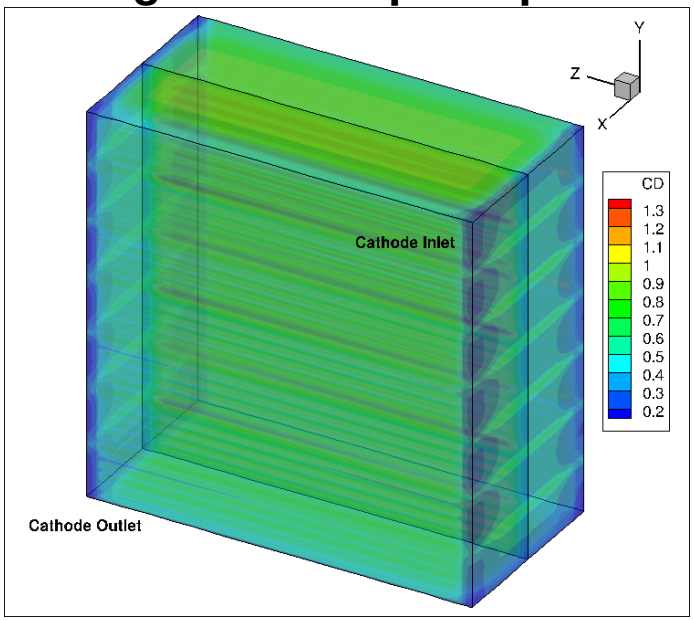
1.0 A/cm^2



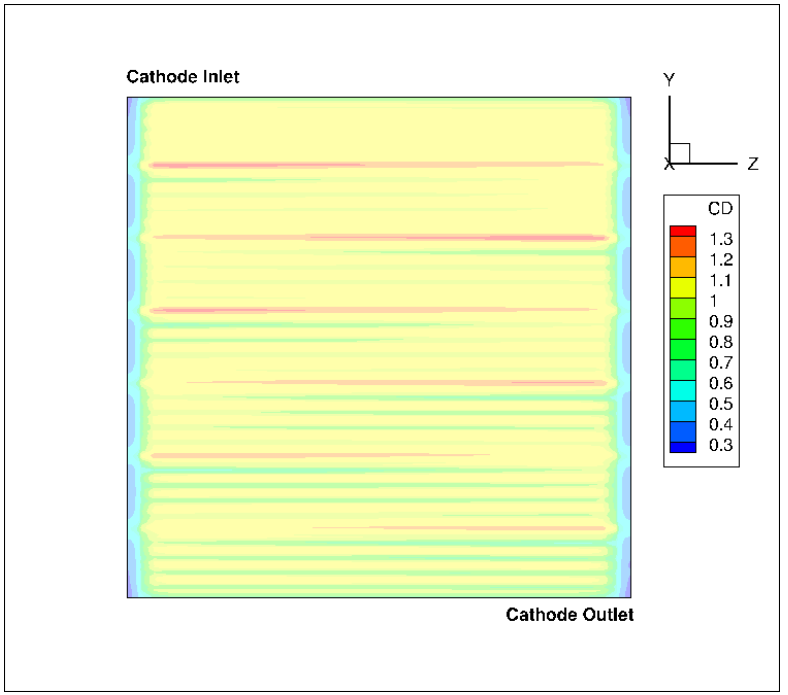
1.2 A/cm^2

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

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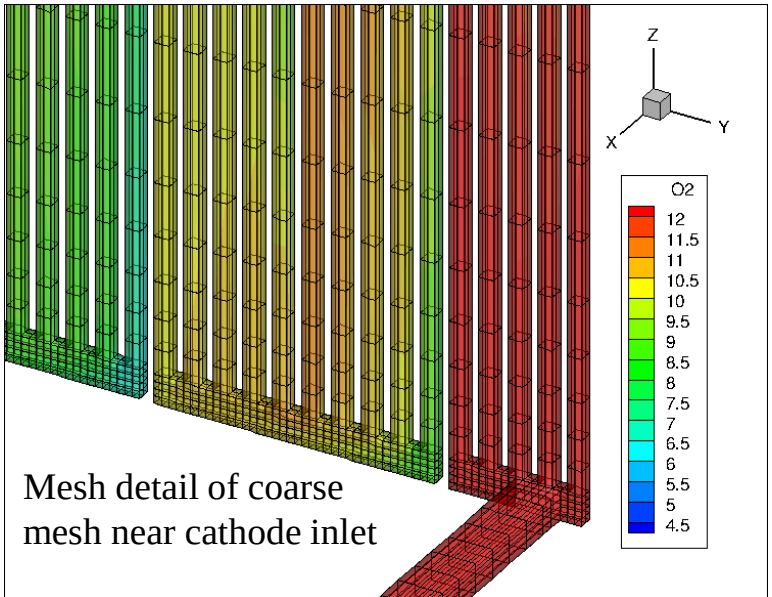
Grid Convergence Study

- **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%

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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

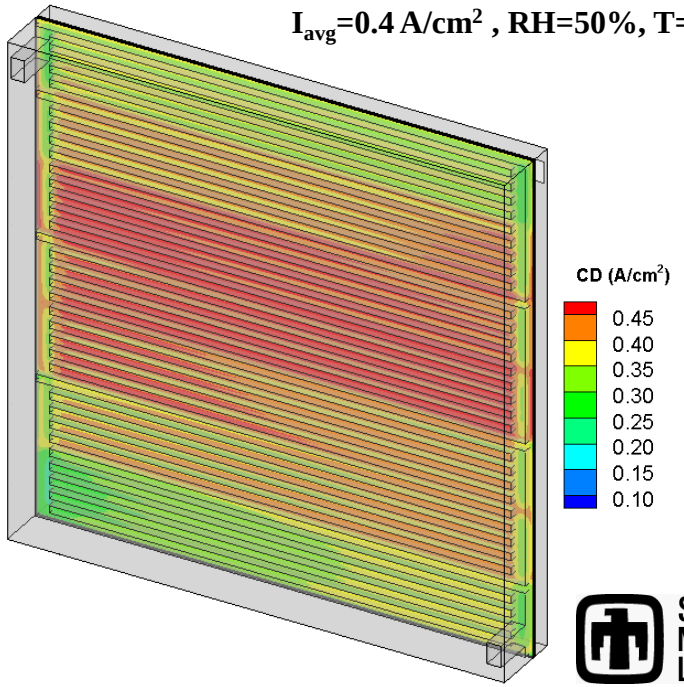
0.0%	19.7%	12.4%	11.3%	12.5%	13.5%	14.7%	13.0%	11.7%	22.7%
-4.2%	5.0%	1.7%	5.1%	5.5%	5.9%	5.4%	3.5%	-1.1%	10.8%
-0.4%	4.0%	4.7%	9.2%	7.5%	7.5%	6.2%	5.2%	-4.4%	6.3%
-7.8%	-3.0%	-0.6%	-2.6%	4.7%	10.0%	10.9%	6.8%	1.4%	13.6%
-3.2%	5.7%	7.4%	4.9%	2.3%	10.2%	13.4%	13.3%	6.9%	13.6%
-1.6%	1.9%	5.6%	5.7%	2.9%	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



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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

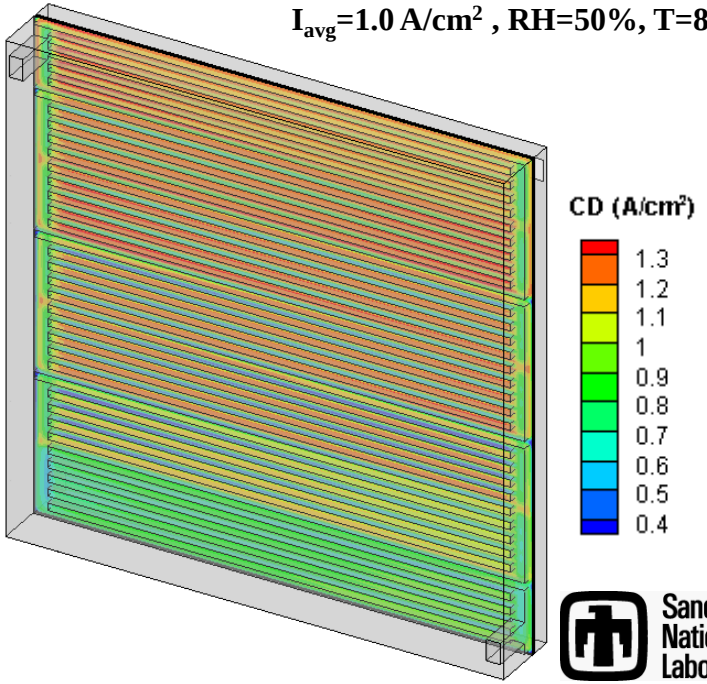
Relative difference between experiments and simulation

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



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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

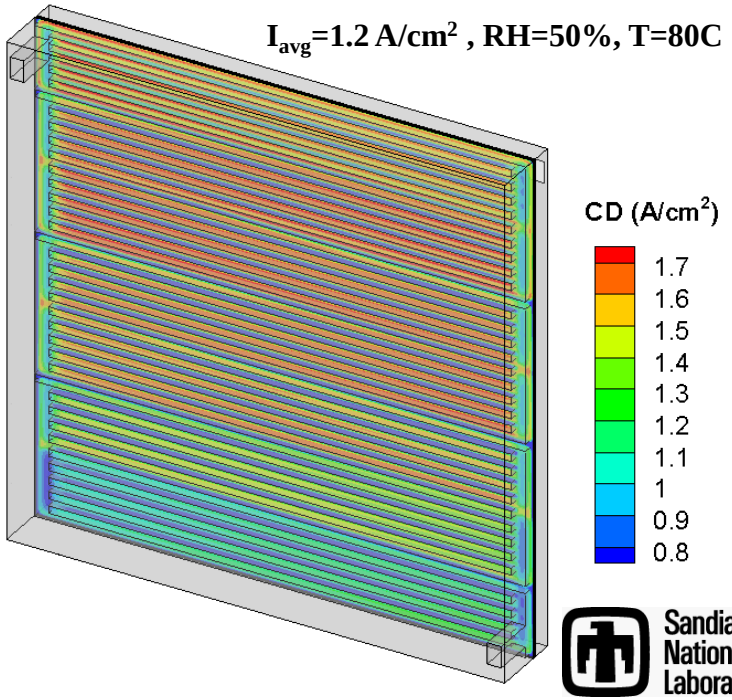
Relative difference between experiments and simulation

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



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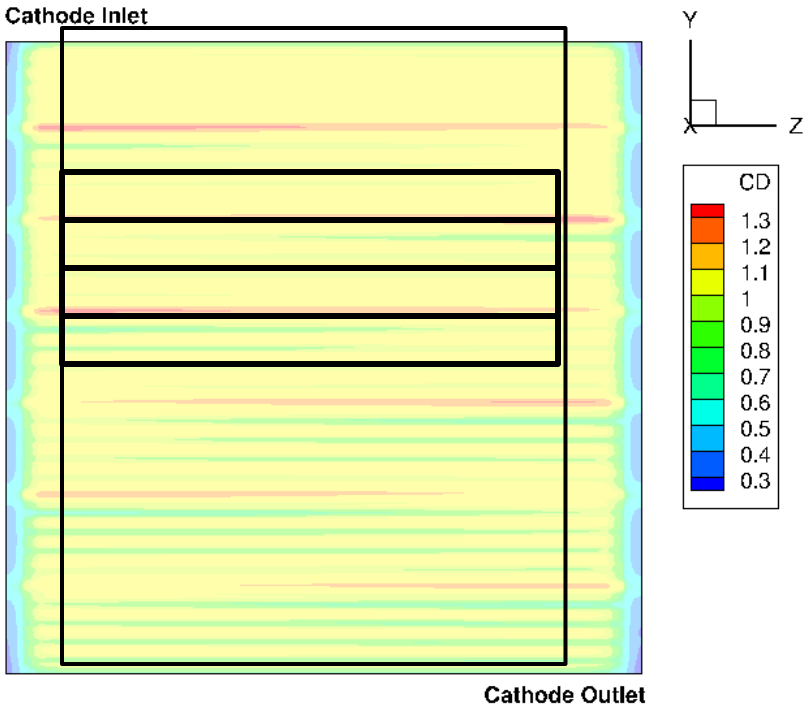
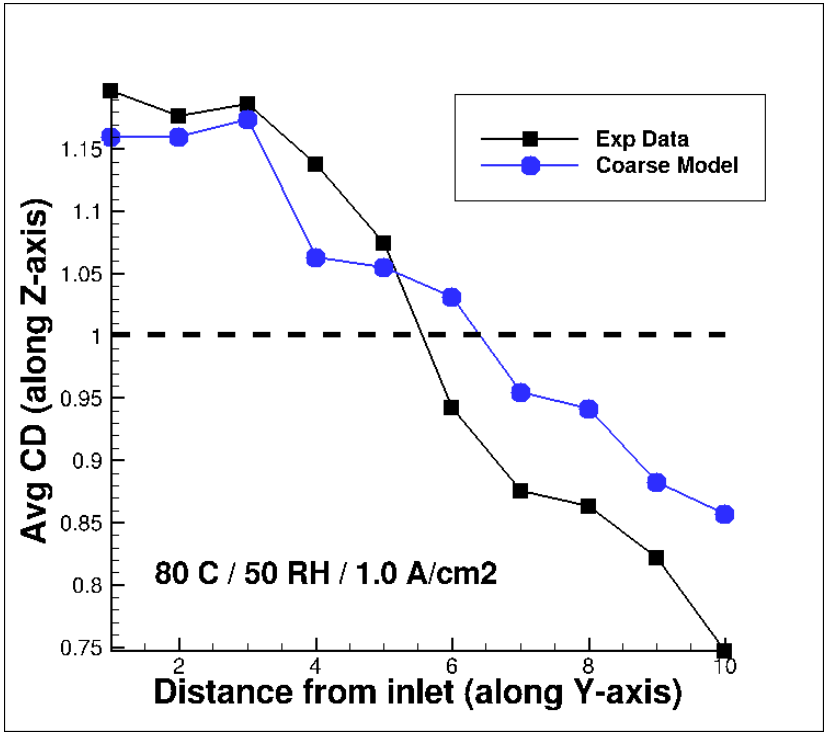
Comparing Local CD Inlet-to-Outlet

- A simpler metric for validation and sensitivity analysis is obtained by averaging the local CD in each row from inlet to outlet
- We exclude the right-/leftmost columns since the current varies widely





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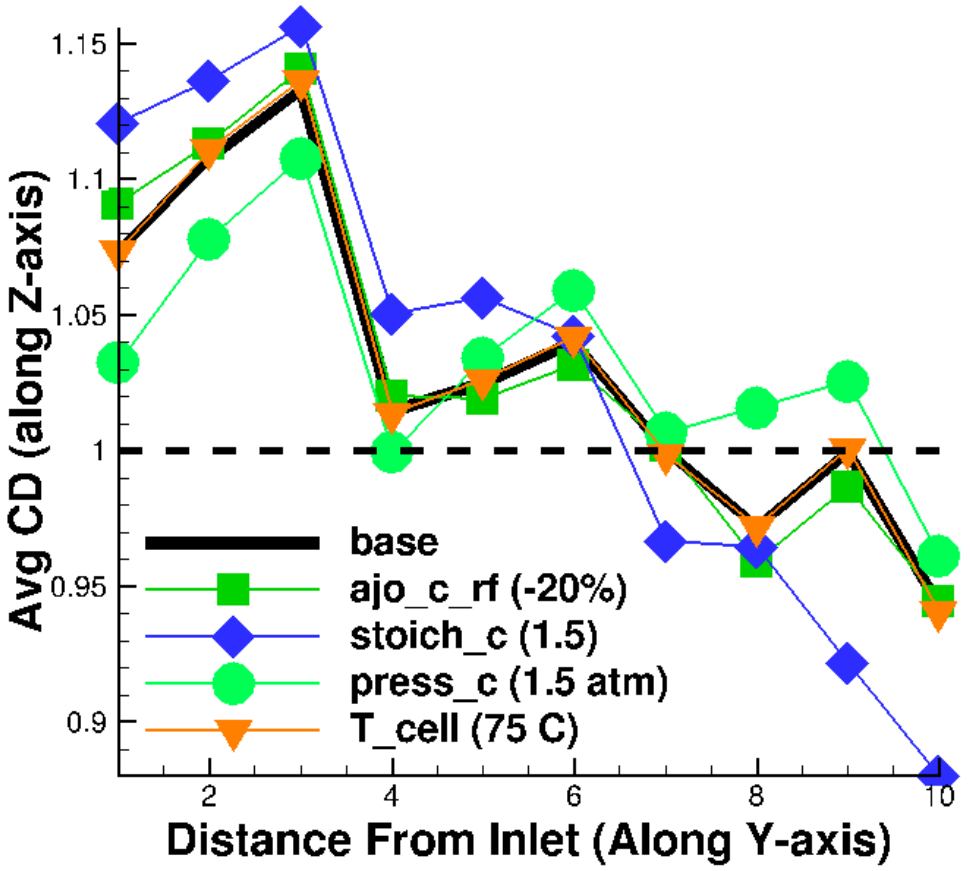
Sensitivity Analysis: Segmented CD

- We studied the effects of a number of parameters on local CD
  - Cathode stoich (1.5-2.5)
  - Cathode reference exchange current (4.8e3 +/- 20%)
  - Cathode back pressure (1-3 atm)
  - Cell temperature (75-85 C)
- Can use partially converged solutions (few 100 iterations)
- We get rough idea of which parameters are most significant for computing local CD



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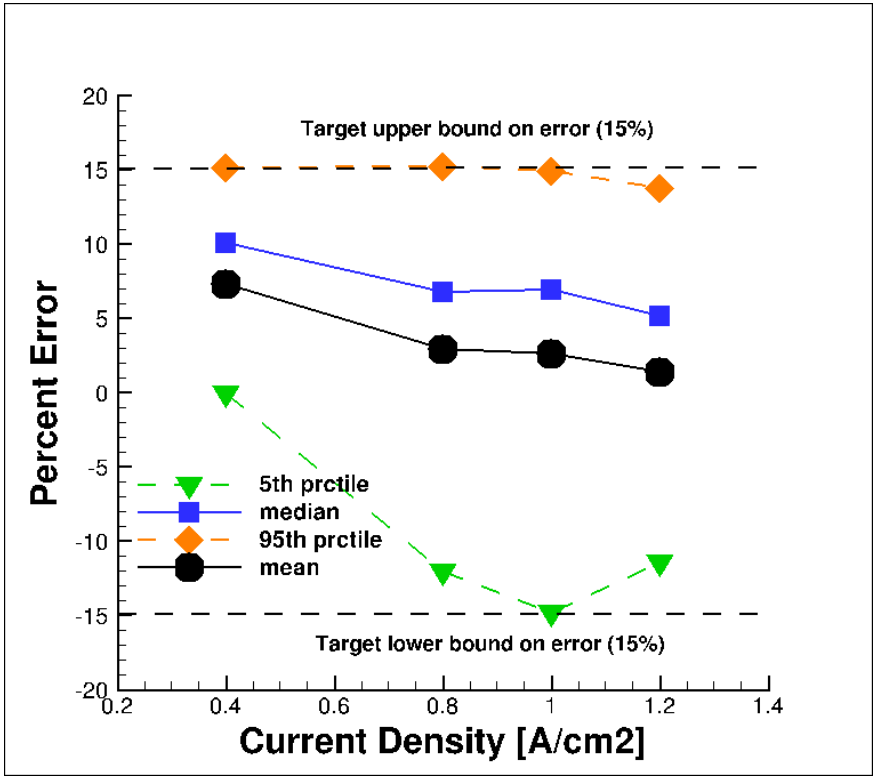
Presenting Validation Using Percentiles

- We are comparing 100 model predictions and experimental data
- It is convenient to exclude outliers and plot the errors within percentiles.
- At the right we summarize the validation data for four different operating CD: 0.4, 0.8, 1.0, and 1.2
- The mean or median error shows a good trend around zero
- The 5th and 95th percentile are within our goal of 15% relative error
- We still need to be concerned with the 10% of points where the relative error may exceed 15%.



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Future Work

- **Further Model Validation**
  - **Complete data set from LANL (60-80 C, 25-50-75-100 RH)**
  - **Using liquid water data from neutron imaging**
  - **Inclusion of two-phase channel model**
  - **Using validation data from partners (Ballard, Nissan)**
- **Short Stack Model Validation**
  - **Multiple channels, multiple cells**

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