AURORA Program

Transport Studies Enabling Efficiency Optimization of Cost-Competitive Fuel Cell Stacks

Presenter: Robert Dross (PM)

Principal Investigator: Amedeo Conti

Nuvera Fuel Cells

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Project ID # **FC028**

Program Overview

Timeline

- Actual start: 9/1/2009
- Planned end: 8/31/2012
- 50% complete

Barriers

- Barriers addressed
  - (B) Cost
  - (C) Performance
  - (E) System thermal & water management

Budget

- Total project funding
  - $4.085 M (DOE)
  - $1.570 M (Cost Share)
- FY'10 Actual funding: $ 1.235 M
- FY'11 Budget funding: $1.050 M

Partners

- Johnson Matthey Fuel Cells
- Penn State University / University of Tennessee
- Lawrence Berkeley Lab

Program Objectives

The **objective** of this program is to optimize the efficiency of a stack technology meeting DOE 2015 cost targets.

Table 3.4.3 Technical Targets: 80-kW$_e$ (net) Transportation Fuel Cell Stacks Operating on Direct Hydrogen [a]					
Characteristic	**Units**	**2003 Status**	**2005 Status**	**2010**	**2015**
Stack power density [b]	W / L	1,330	1,500 [c]	2,000	2,000
Stack specific power	W / kg	1,260	1,400 [c]	2,000	2,000
Stack efficiency [d] @ 25% of rated power	%	65	65	65	65
Stack efficiency [d] @ rated power	%	55	55	55	55
Cost[e]	\$ / kW$_e$	200	70 [f]	25	15
Durability with cycling	hours	N/A	2,000 [g]	5,000 [h]	5,000 [h]

[e] Based on 2002 dollars and cost projected to high-volume production (500,000 stacks per year).

<u>Program is on schedule and the 2010 Go/No-Go milestone has been met</u>

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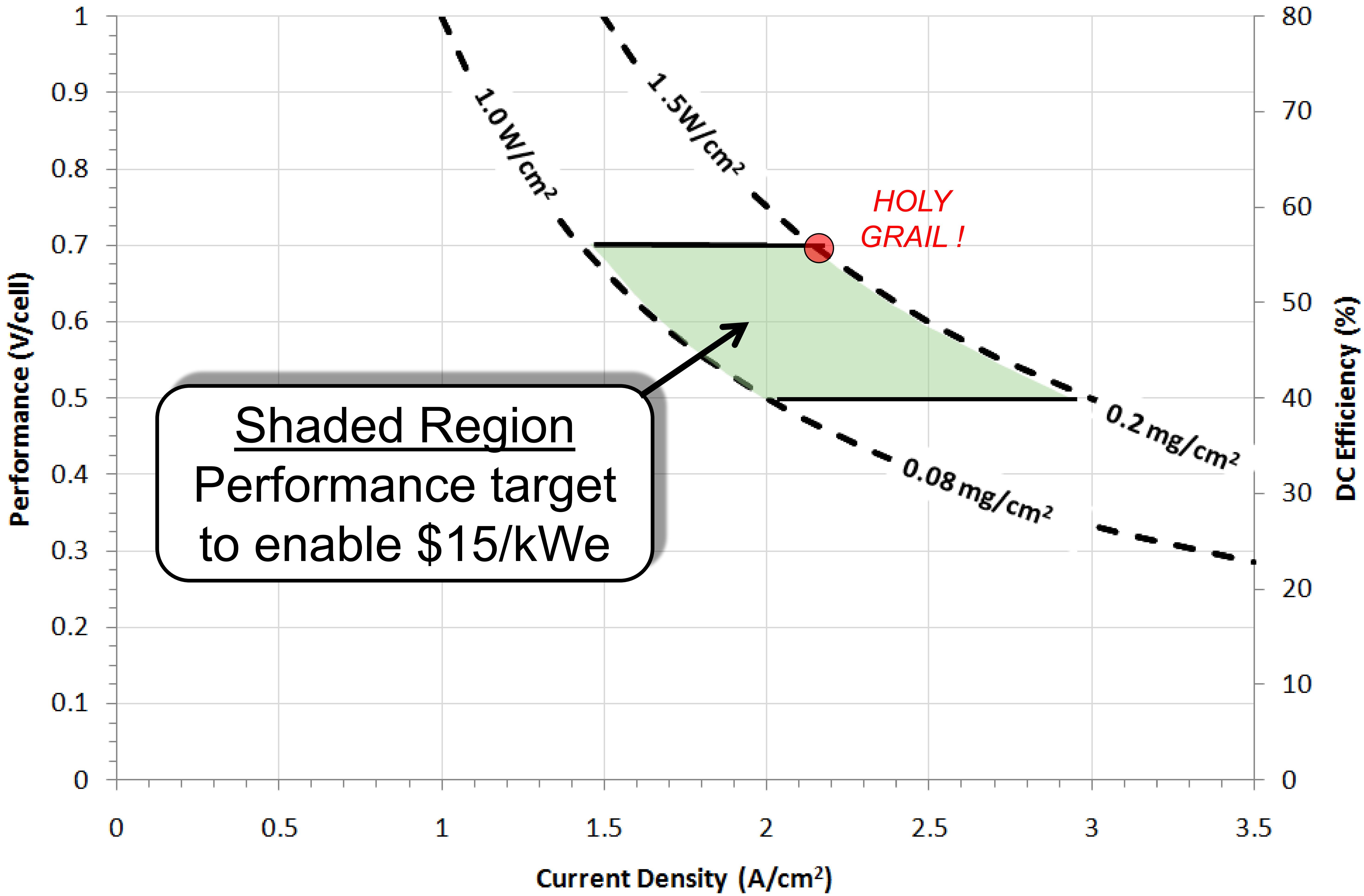
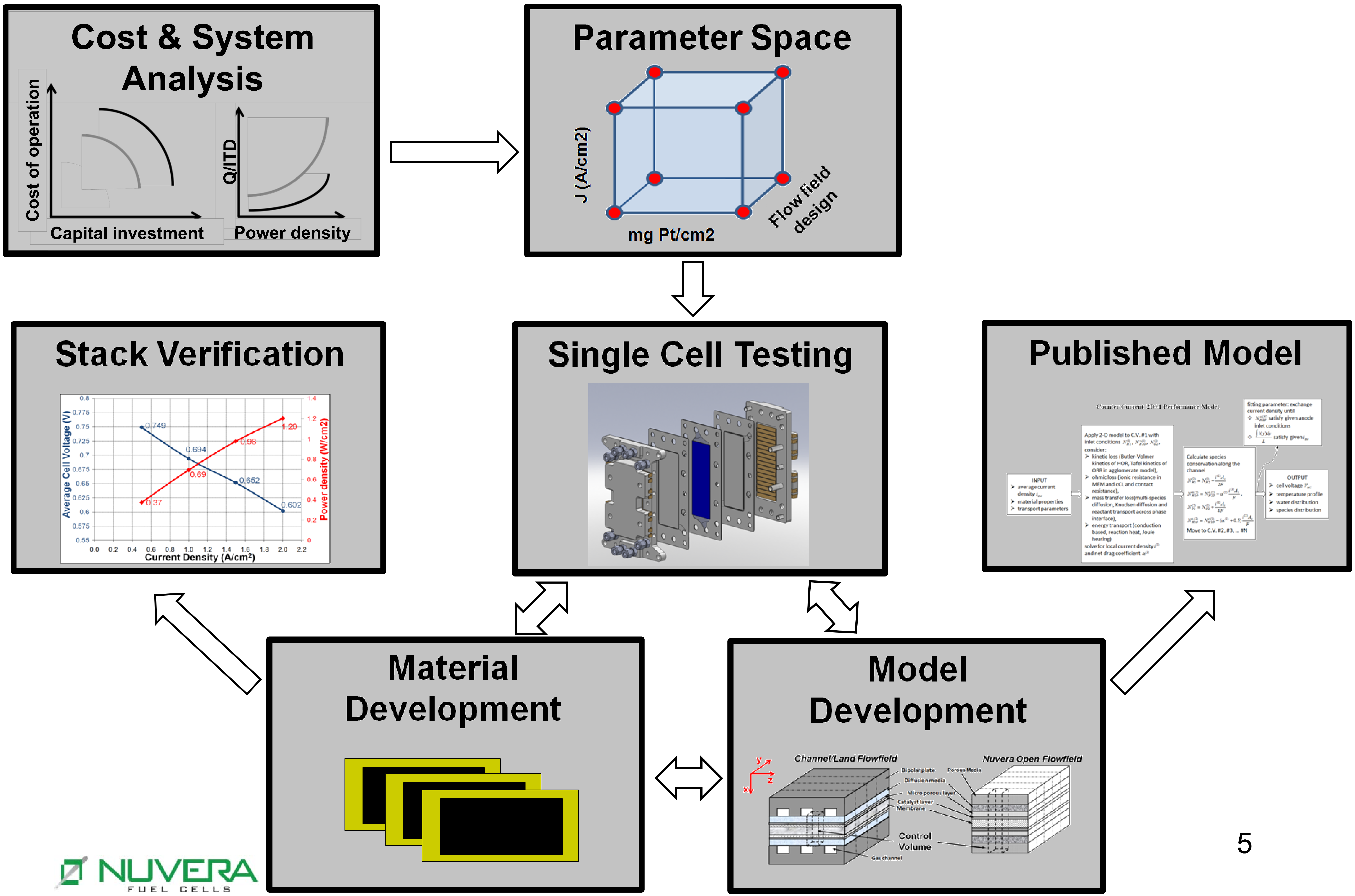
Technical Target - Approach

Target: Demonstrate stable and repeatable high power performance on a full format fuel cell stack: 7.5 W/mg-Pt @ 500mV.

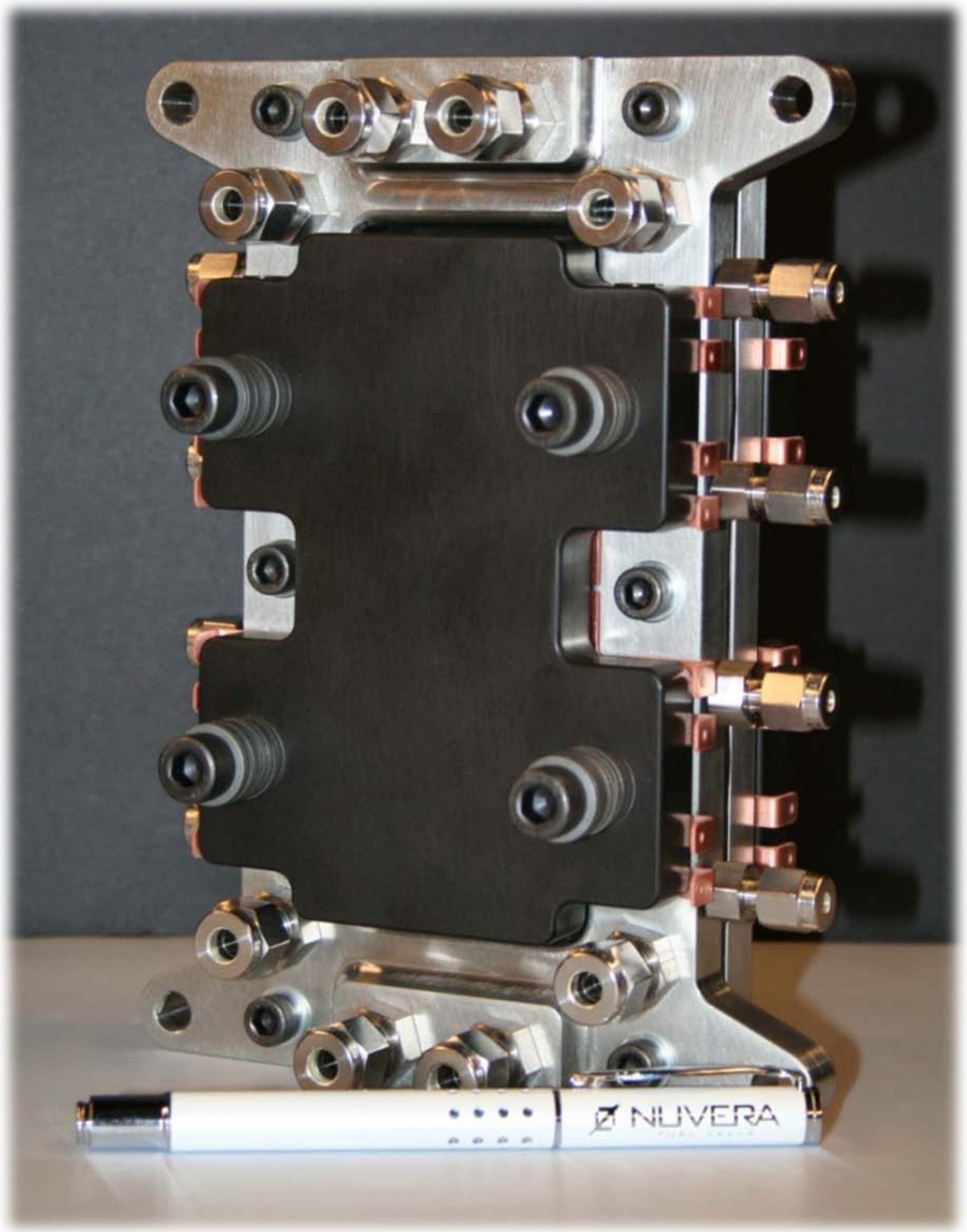


Program Approach

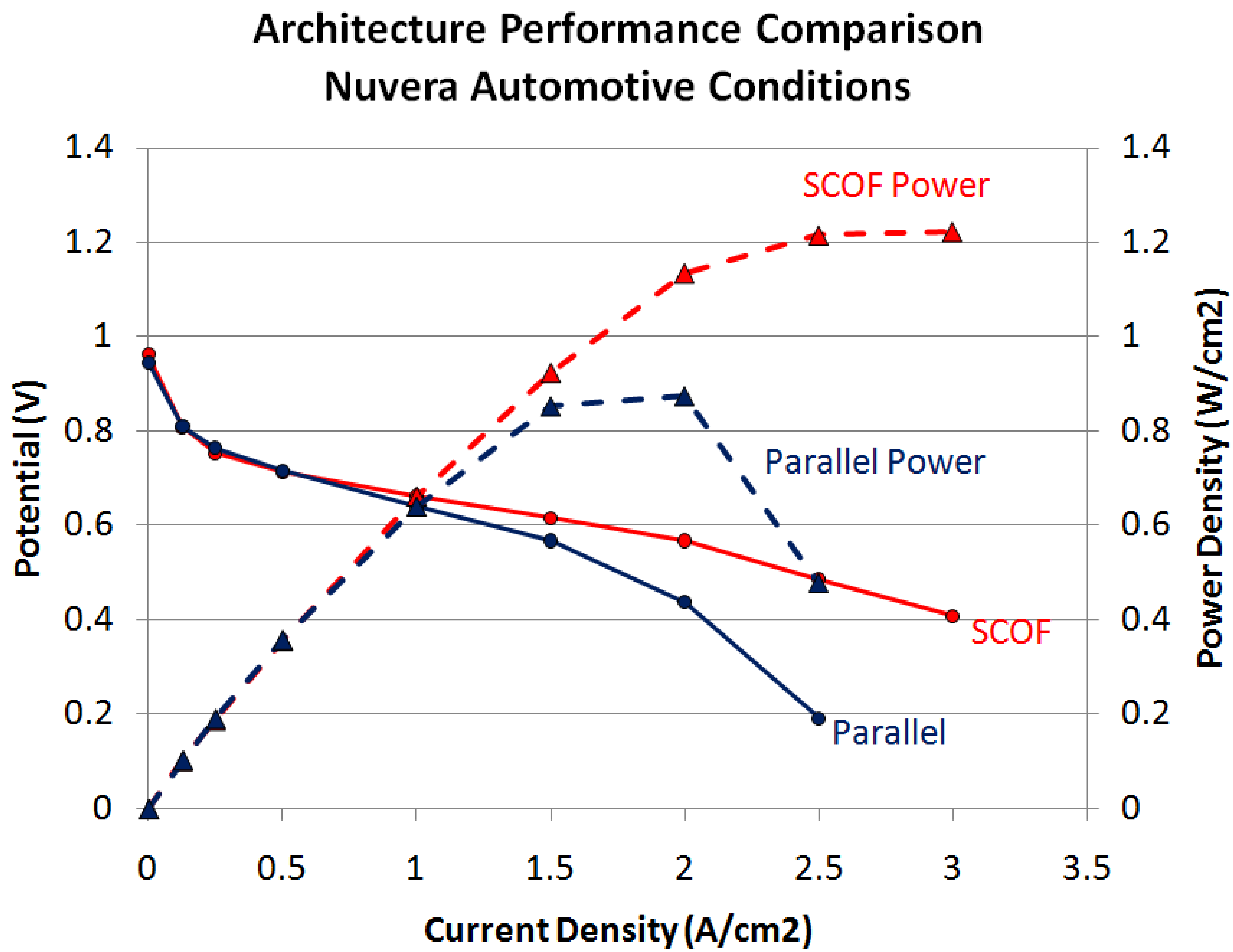


Single Cell Testing

Single cell testing demonstrates the motivation to investigate ultra-high current densities with the open flowfield architecture.



Single Cell Open Flowfield (SCOF) Hardware



T_{cell}= 60 °C, An 50% RH, Ca 0% RH, Press ~1.1 to 1.8 bara
MEA: Gore 5730, 0.15 mg Pt/cm^2 An, 0.4 mg Pt/cm^2 Ca
GDL: SGL 25BC

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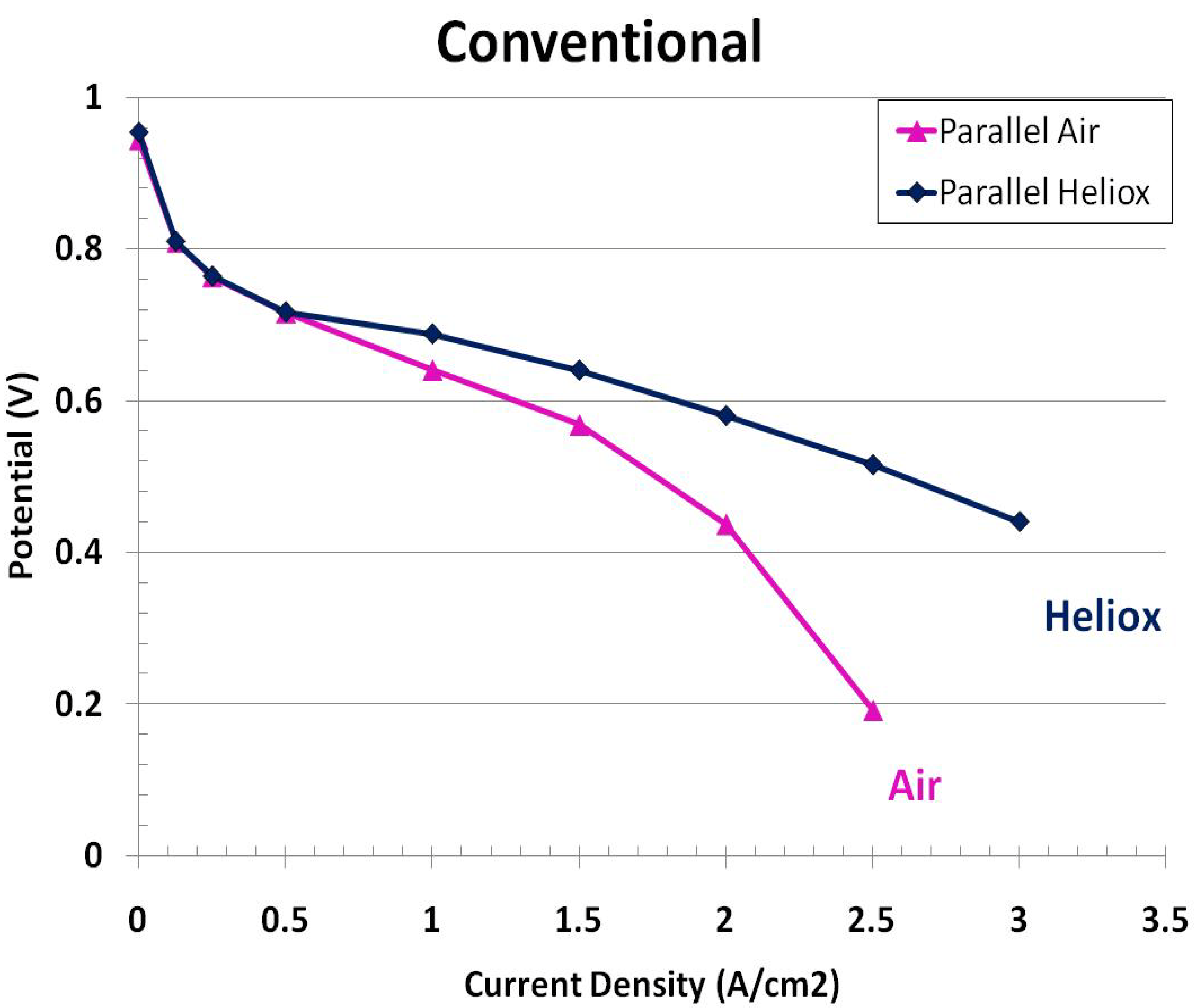
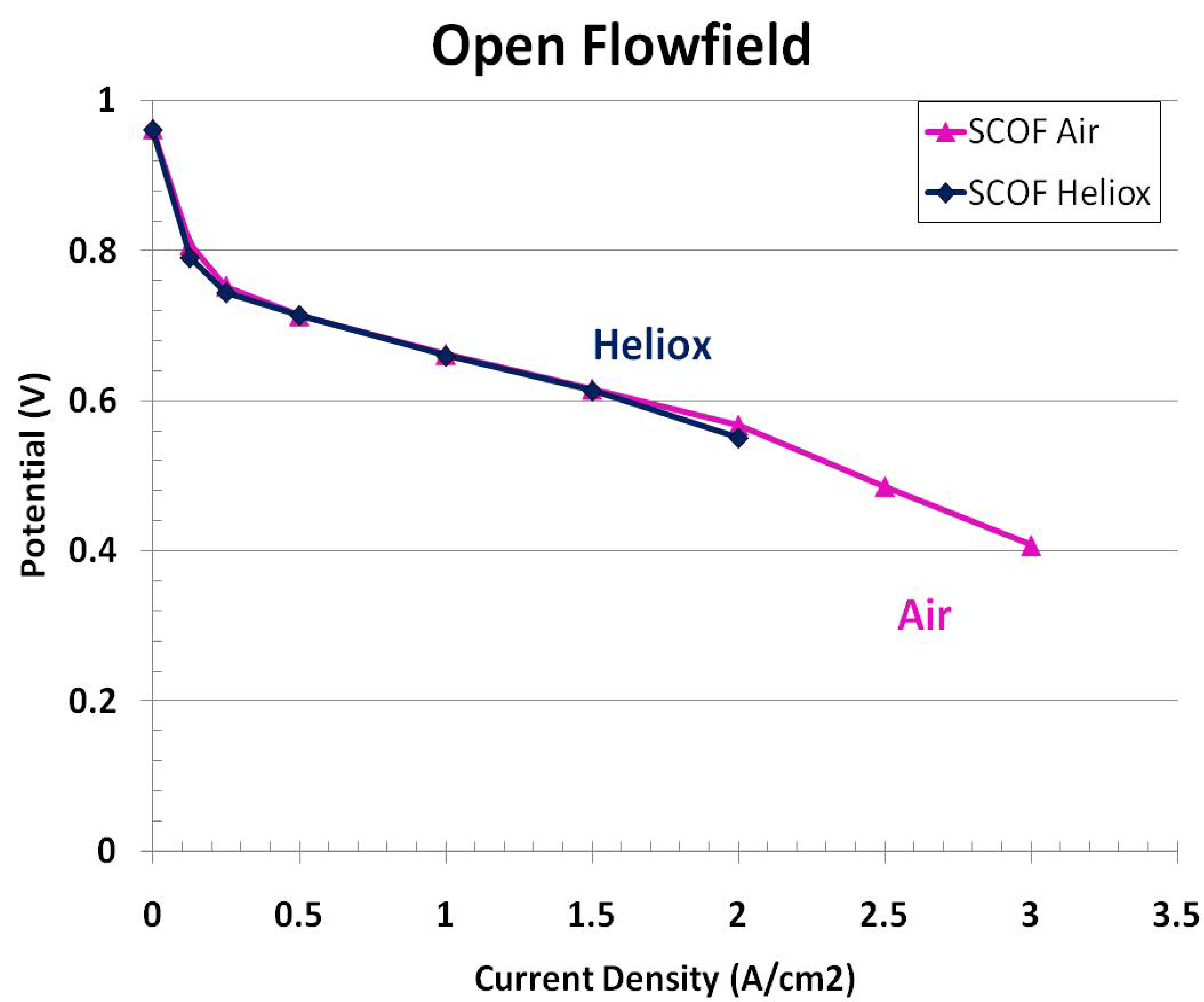
Transport Studies

Diagnostic testing has been conducted to study transport phenomena at ultra-high current densities.





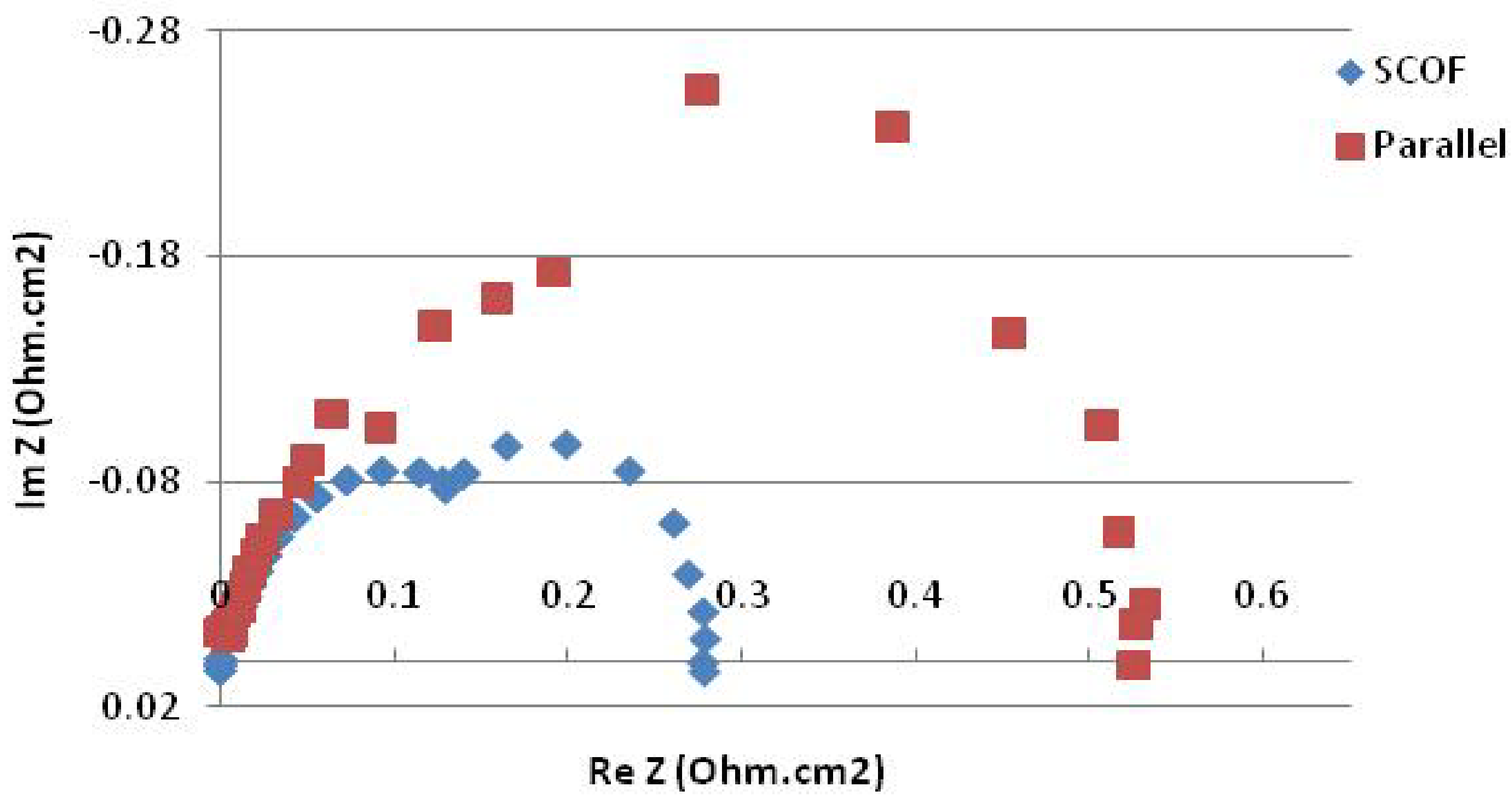
These type of data provide essential input to the detailed transport model

T_{cell}= 60 °C, An 50% RH, Ca 0% RH, Press ~1.1 to 1.8 bara
MEA: Gore 5730, 0.15 mg Pt/cm^2 An, 0.4 mg Pt/cm^2 Ca
GDL: SGL 25BC

Transport Studies

EIS testing confirms a difference in mass transport resistance between channel/land and open flowfield architectures.

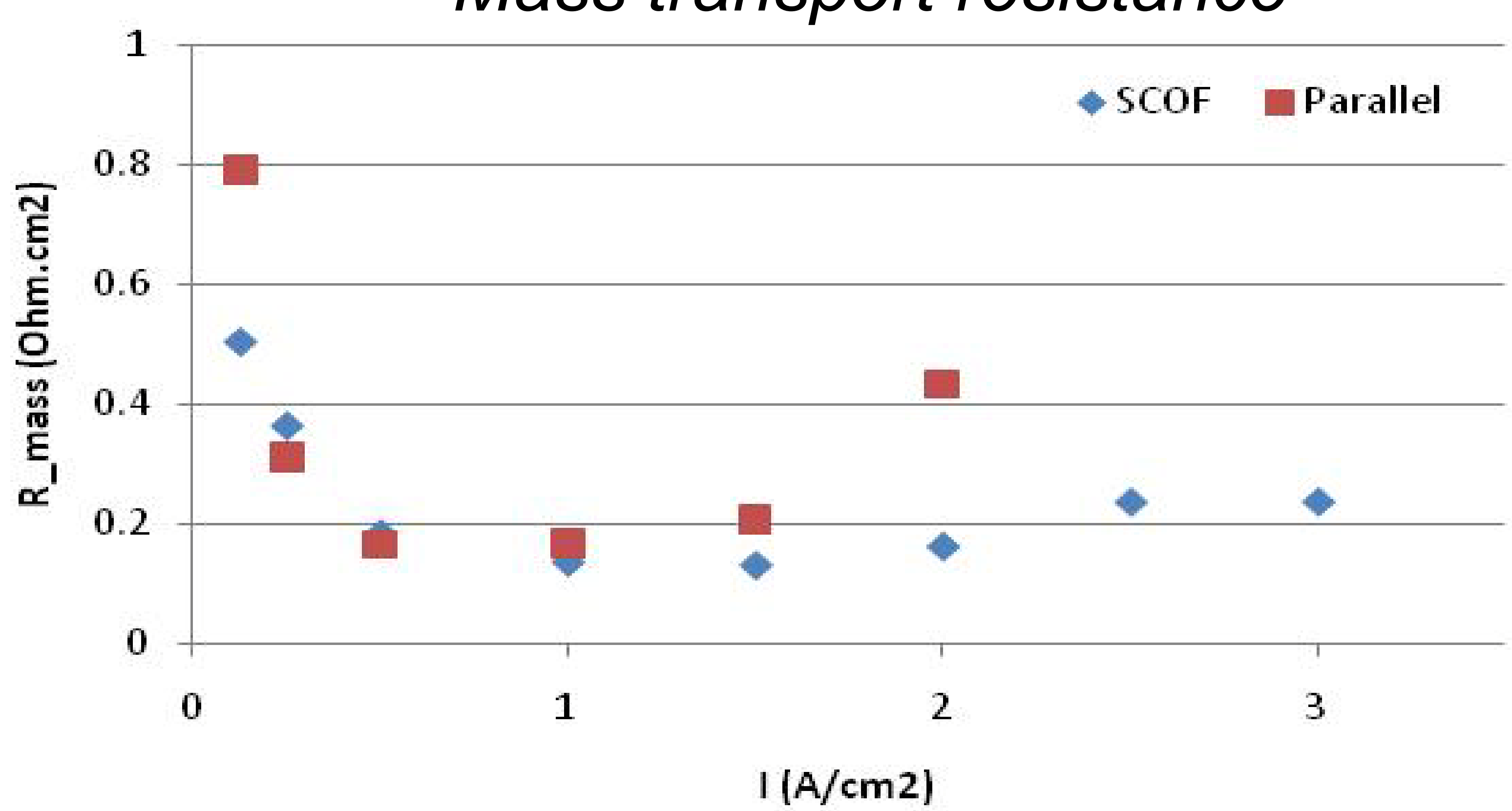
***iR Free** Nyquist plots, 2 A/cm² - SCOF vs Parallel*



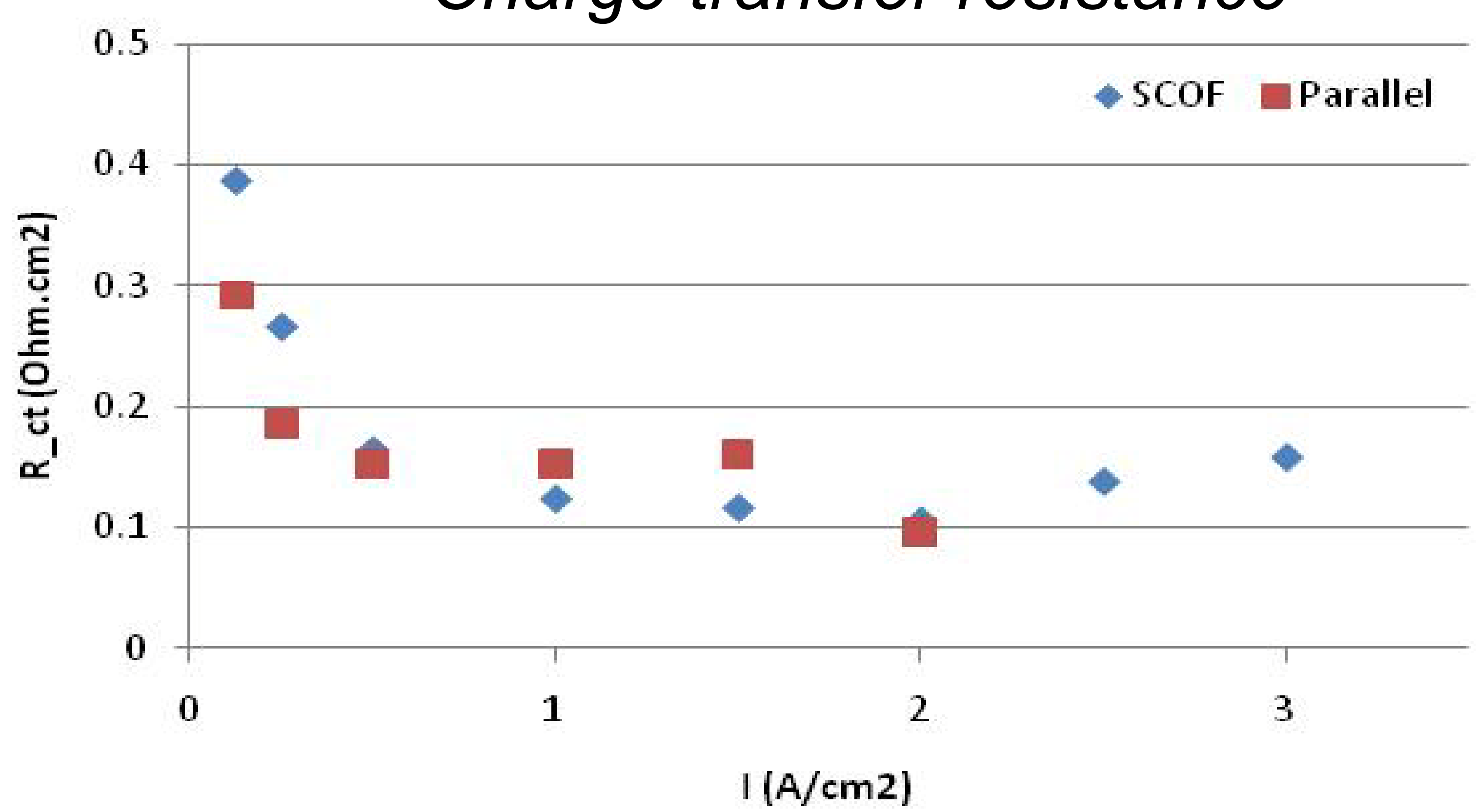
Test Conditions

T_{cell}= 60 ºC, An RH 50%, Ca RH 0%, Press ~1.1 to 1.8 bara
MEA: Gore 5730, 0.15 mg Pt/cm^2 An, 0.4 mg Pt/cm^2 Ca
GDL: SGL 25BC

Mass transport resistance



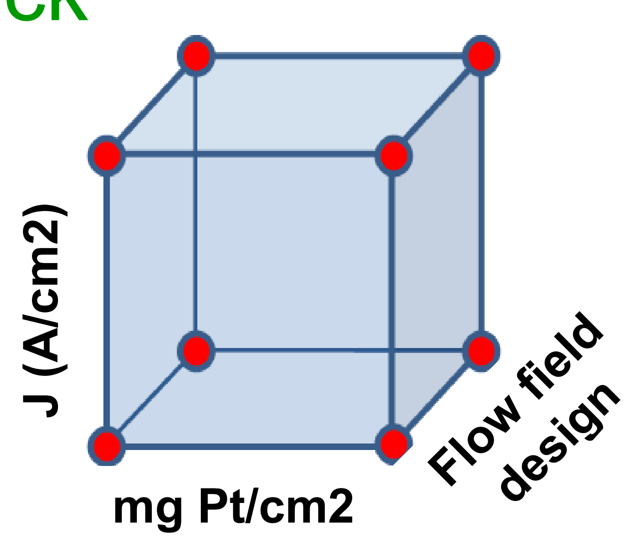
Charge transfer resistance



Model Roadmap

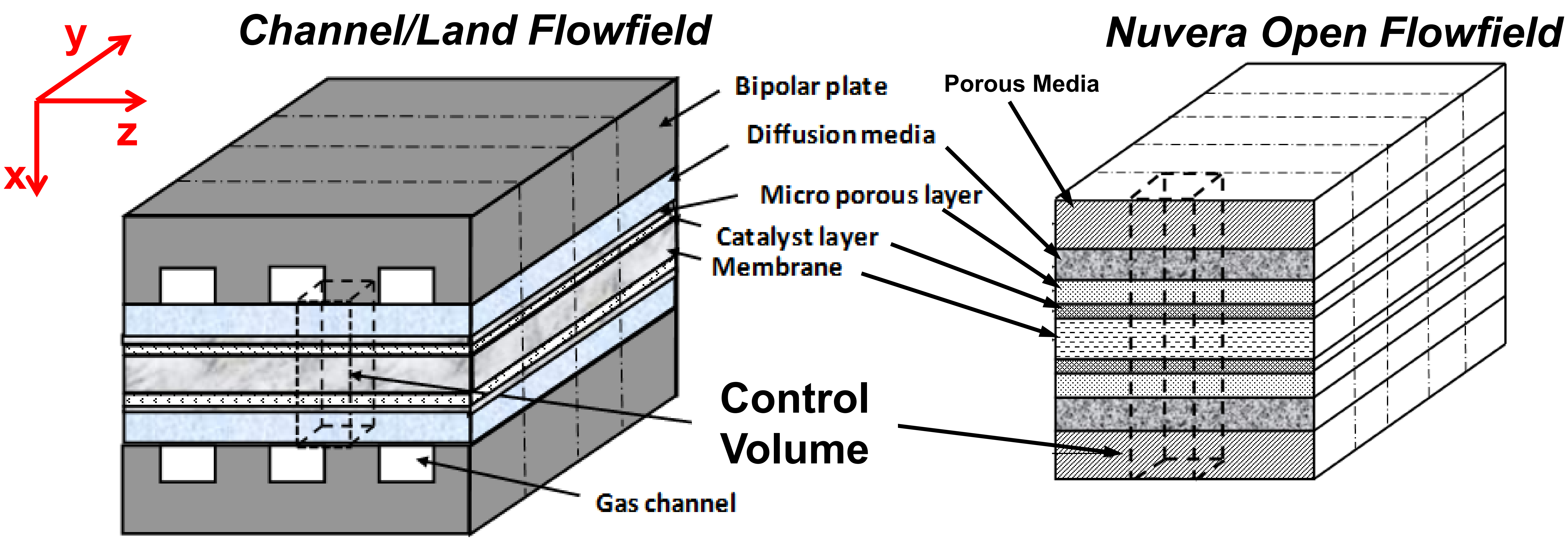
A model capable of predicting high current density operation in different architectures is the central deliverable of the program

- **Single phase model generation** from PSU 2D channel/land model – **Q2 2010** Completed
  - 2D +1, counter flow reactants, compatible with multiple architectures
- **Initial validation with empirical Nuvera model – Q3 2010** Completed
- **Initial performance verification** – **Q4 2010** Completed
- **Multi-phase physics implementation** – **Q1 2011** Completed
  - Verification with empirical Nuvera model
  - Initial performance verification
- **Agglomerate electrode model implementation (LBNL)** – **Q1 2011** Completed
- **Tune model parameters and collect dataset – Q3 2011** On Track
  - Test various architectures and MEA designs (Pt loading, membrane thickness, ionomer EW, etc…)
  - Feedback: Performance, Water Balance, Current Density Distribution
- **Model Validation**: Demonstrate predictive capability – **Q4 2011** On Track
- **Model Publication** – **Q3 2012** On Track



FC Modeling -- Approach

The physics of the quasi-3D, multi-architecture model will be as similar as possible between channel/land and open flowfields.



2D+1 model reduces computational efforts

- No parameters vary in Y direction inside control volume.
- Species concentrations and T vary in Y direction along different control volumes.
- 2D model (XZ) is inferred by variations along Y and uses a fine mesh to predict local conditions accurately.

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FC Modeling -- Approach

Block diagram

Counter-Current 2D+1 Performance Model

INPUT
- average current density i_{ave}
- material properties
- transport parameters

Apply 2-D model to C.V. #1 with inlet conditions $N_{H2}^{(1)}$, $N_{H2O}^{c,(1)}$, $N_{O2}^{(1)}$, consider:
- kinetic loss (Butler-Volmer kinetics of HOR, Tafel kinetics of ORR in agglomerate model),
- ohmic loss (ionic resistance in MEM and cCL and contact resistance),
- mass transfer loss(multi-species diffusion, Knudsen diffusion and reactant transport across phase interface),
- energy transport (conduction based, reaction heat, Joule heating)

solve for local current density $i^{(1)}$ and net drag coefficient $\alpha^{(1)}$

Calculate species conservation along the channel

$$N_{H2}^{(2)} = N_{H2}^{(1)} - \frac{i^{(1)} A_s}{2F}$$

$$N_{H2O}^{a,(2)} = N_{H2O}^{a,(1)} - \alpha^{(1)} \frac{i^{(1)} A_s}{F},$$

$$N_{O2}^{(2)} = N_{O2}^{(1)} + \frac{i^{(1)} A_s}{4F}$$

$$N_{H2O}^{c,(2)} = N_{H2O}^{c,(1)} - (\alpha^{(1)} + 0.5) \frac{i^{(1)} A_s}{F}$$

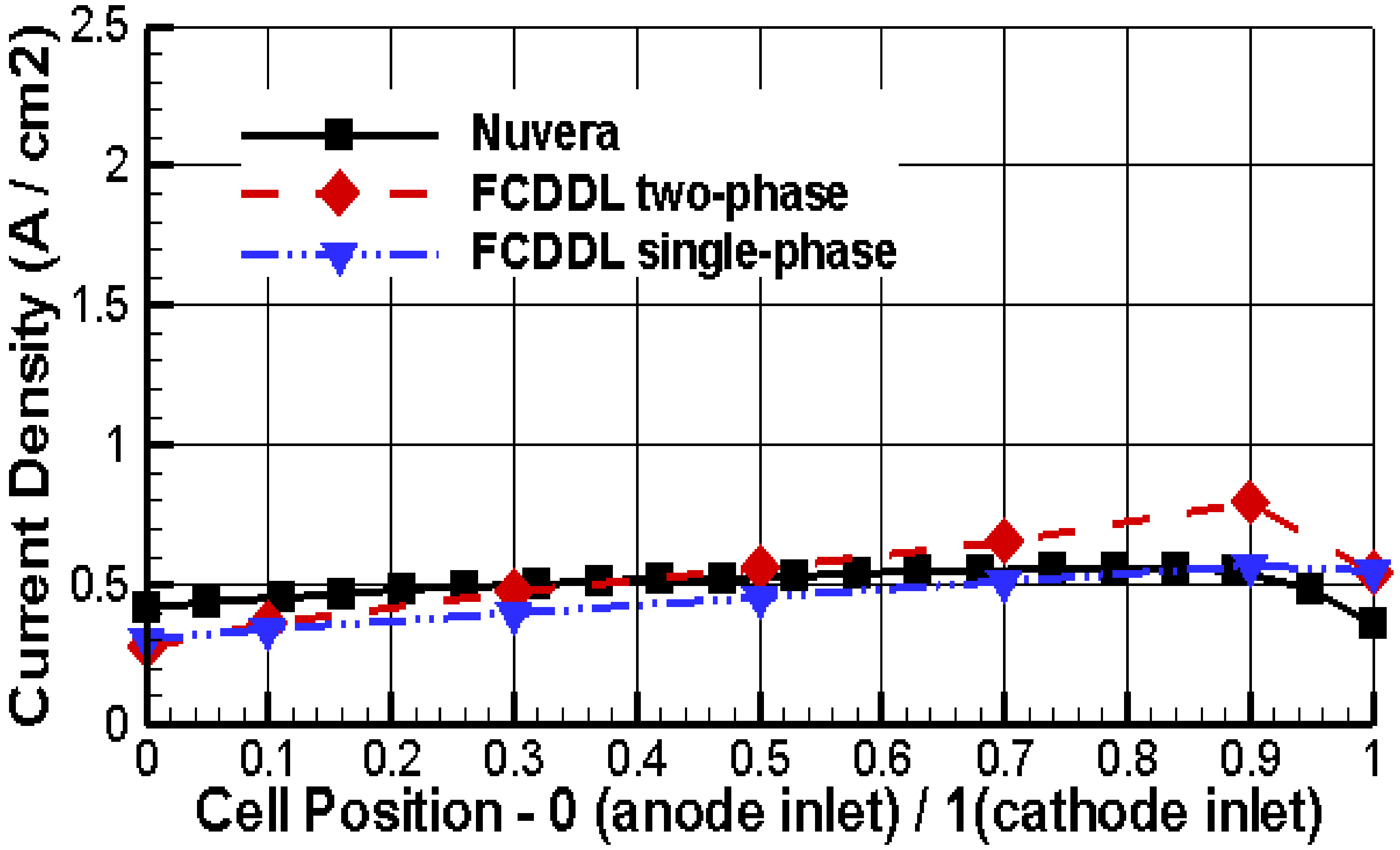
Move to C.V. #2, #3, ... #N

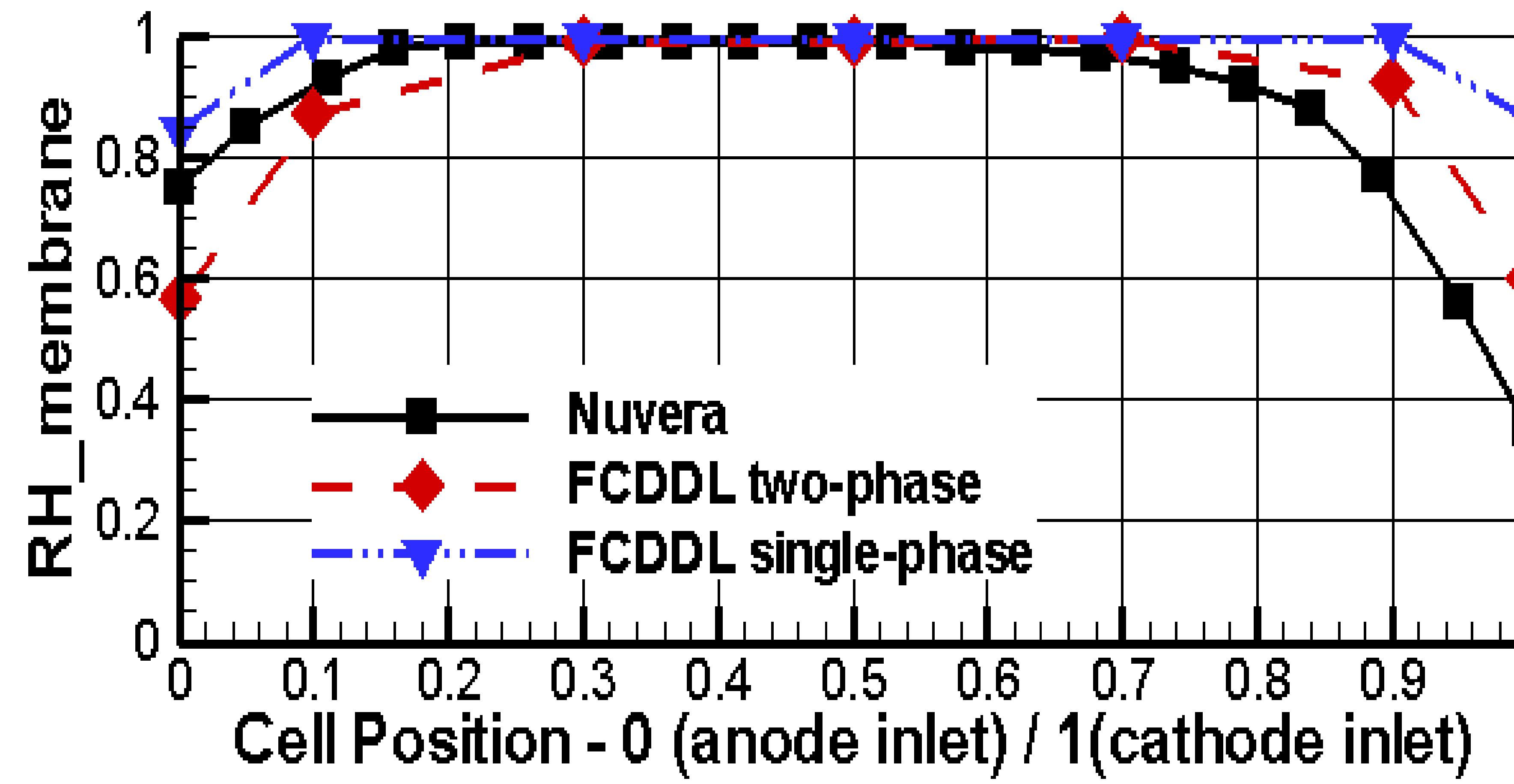
fitting parameter: exchange current density until
- $N_{H2O}^{a,(N)}$ satisfy given anode inlet conditions
- $\frac{\int i(y)dy}{L}$ satisfy given i_{ave}

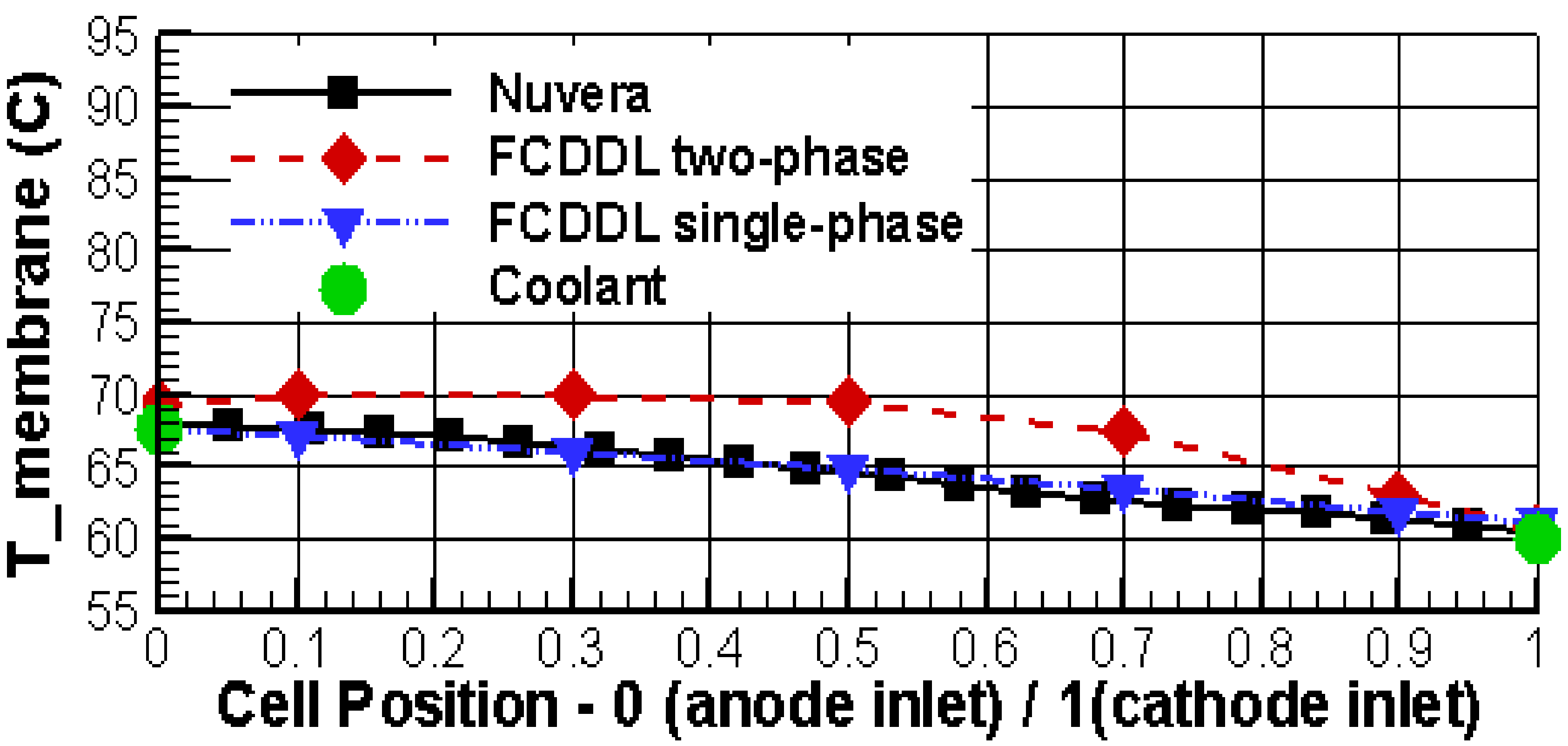
OUTPUT
- cell voltage V_{cell}
- temperature profile
- water distribution
- species distribution

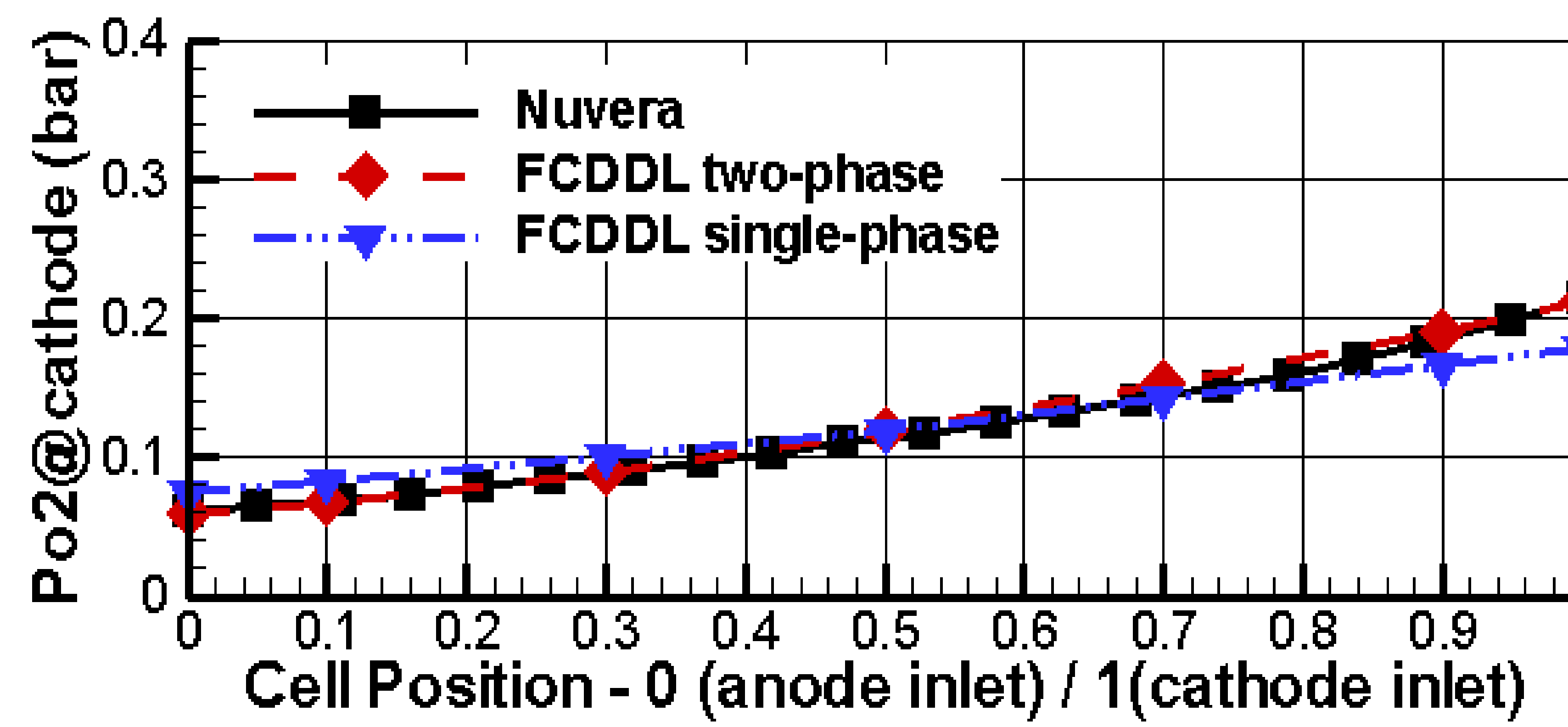
FC Modeling - Status

Agreement with Nuvera empirical model was achieved with both single-phase and two-phase models.





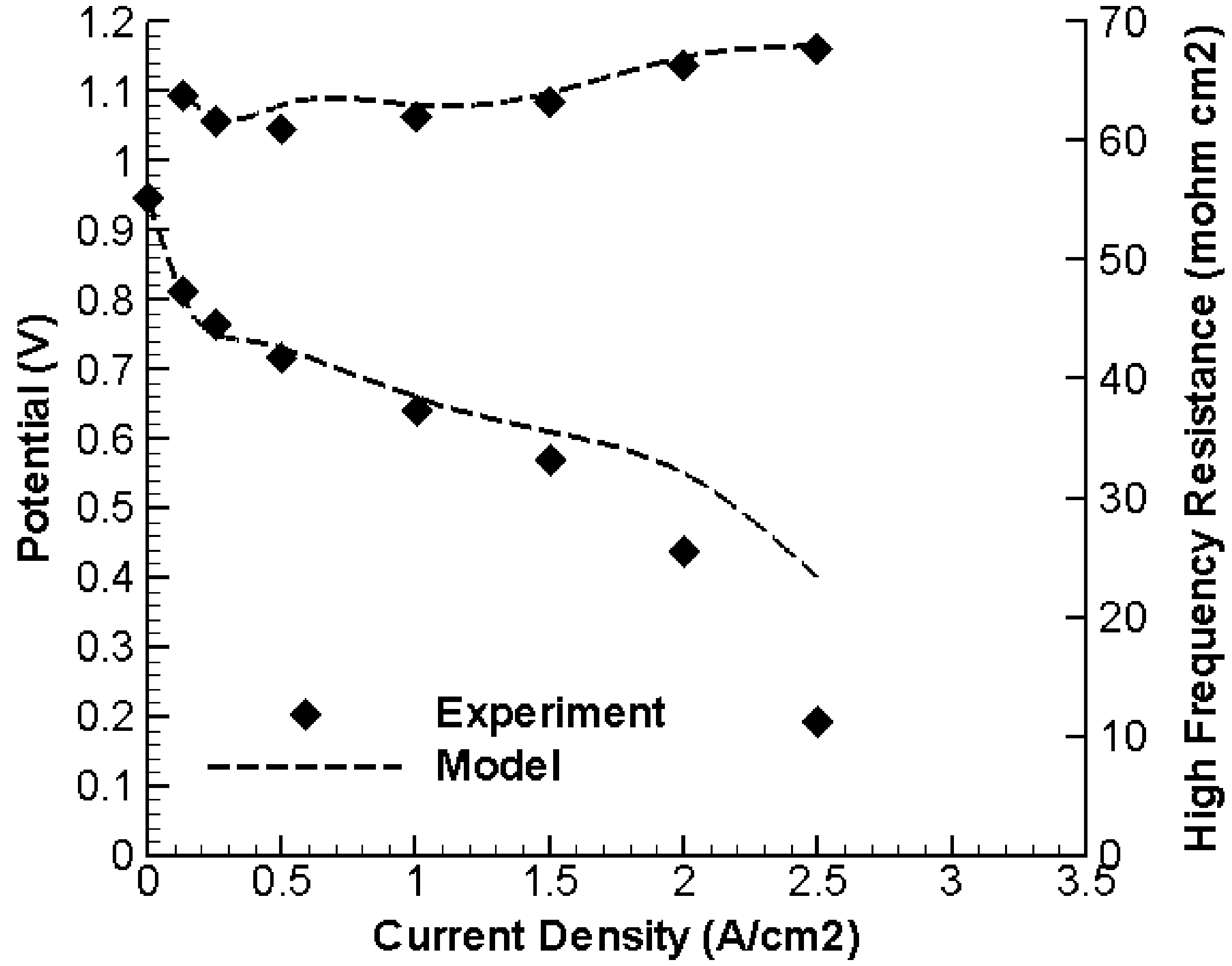




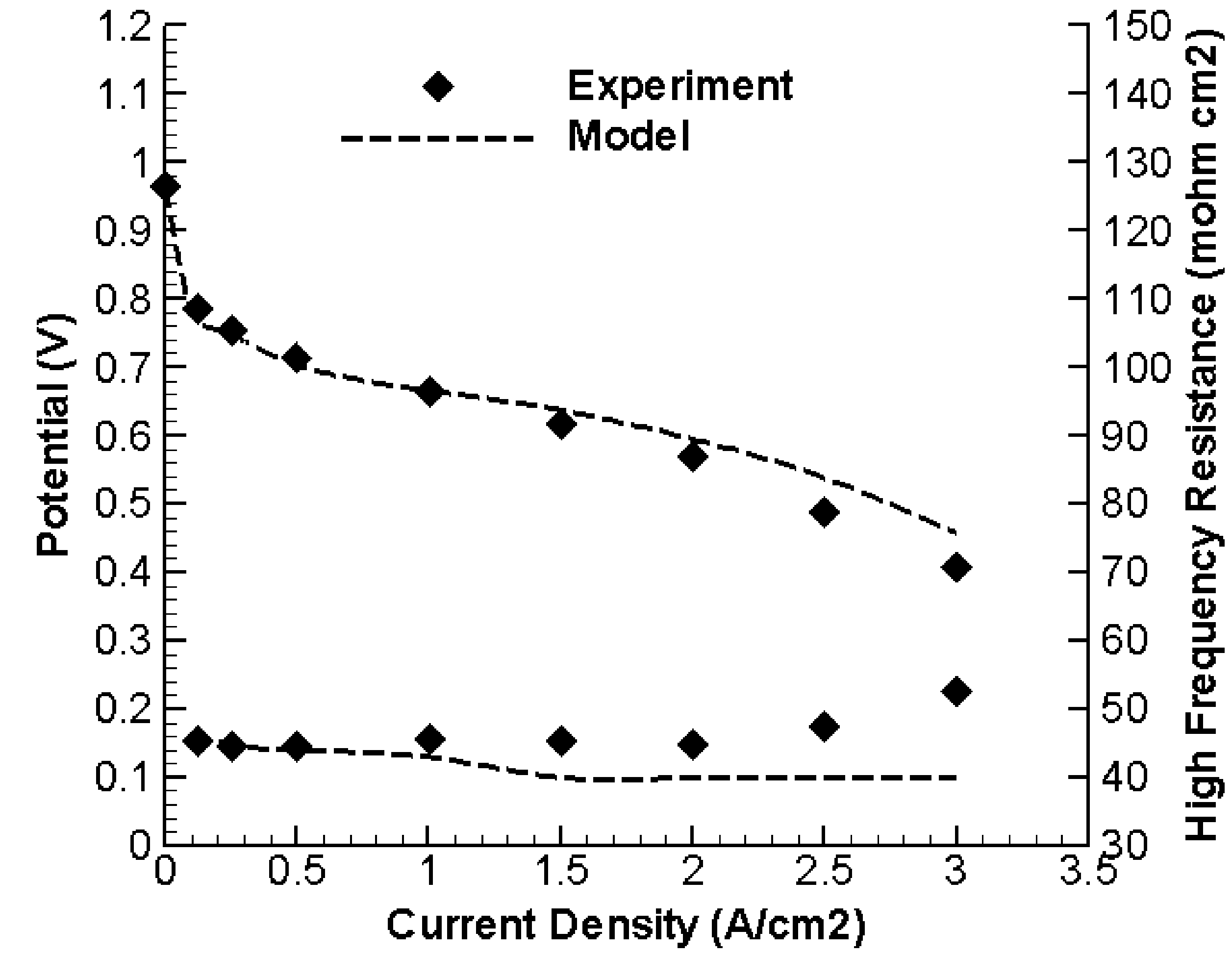
FC Modeling - Status

Initial model verification for both conventional and open flowfield architectures has been conducted.

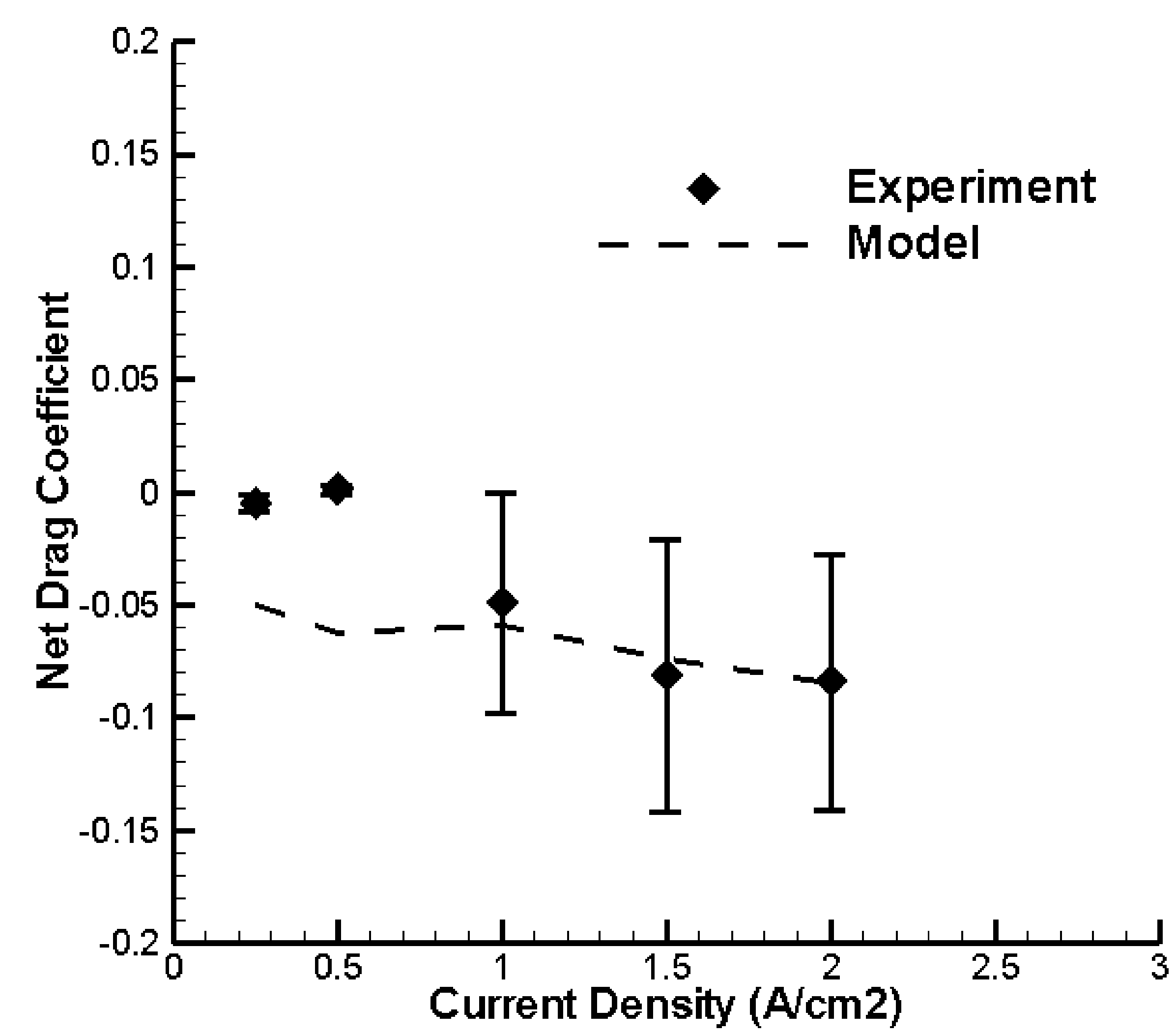
Conventional



Open Flowfield

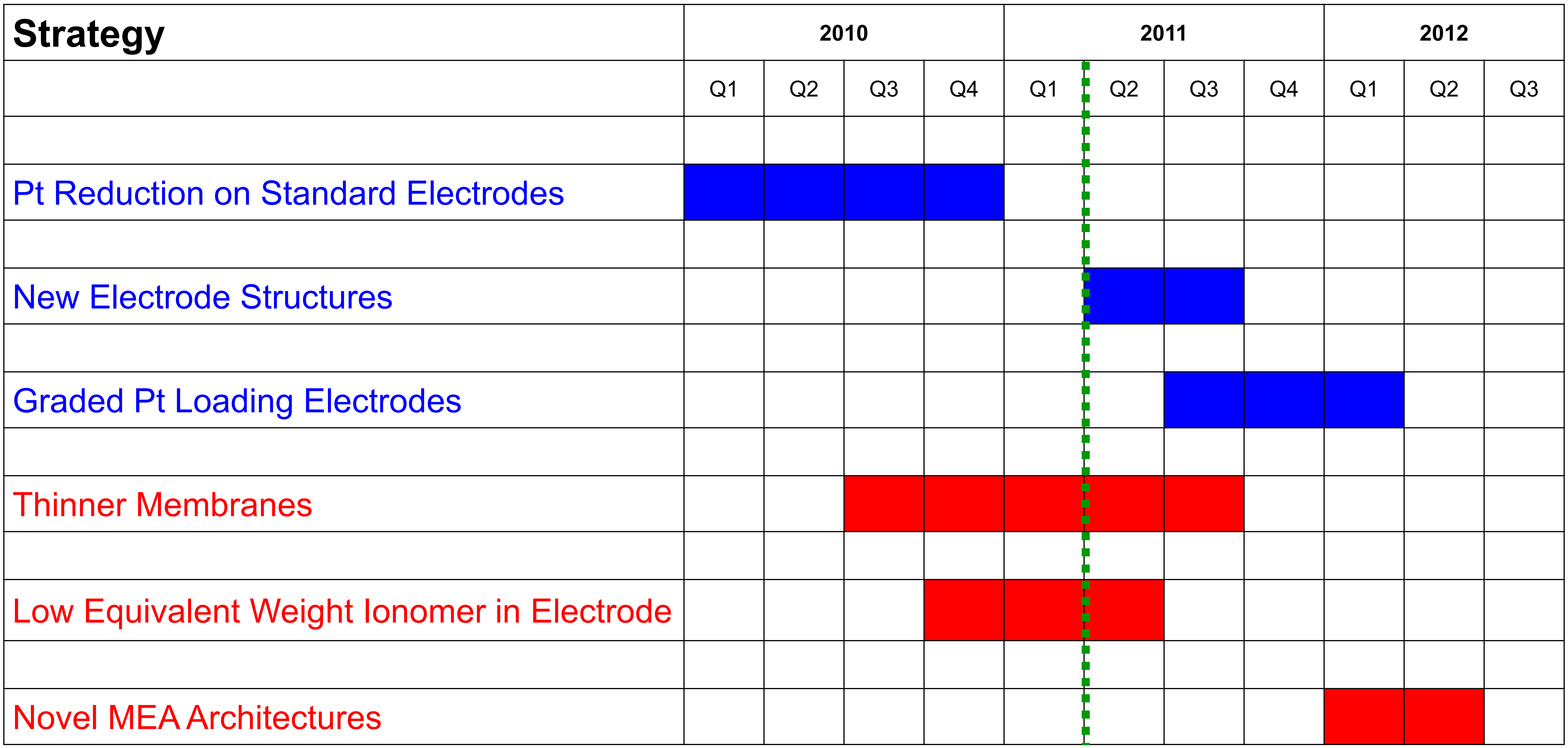


- Initial model verification has been conducted for both architectures showing good correlation
- Some deviation occurs, especially in the ultra-high current density regime
- Model tuning will continue and the final model validation is scheduled for Q4 2011



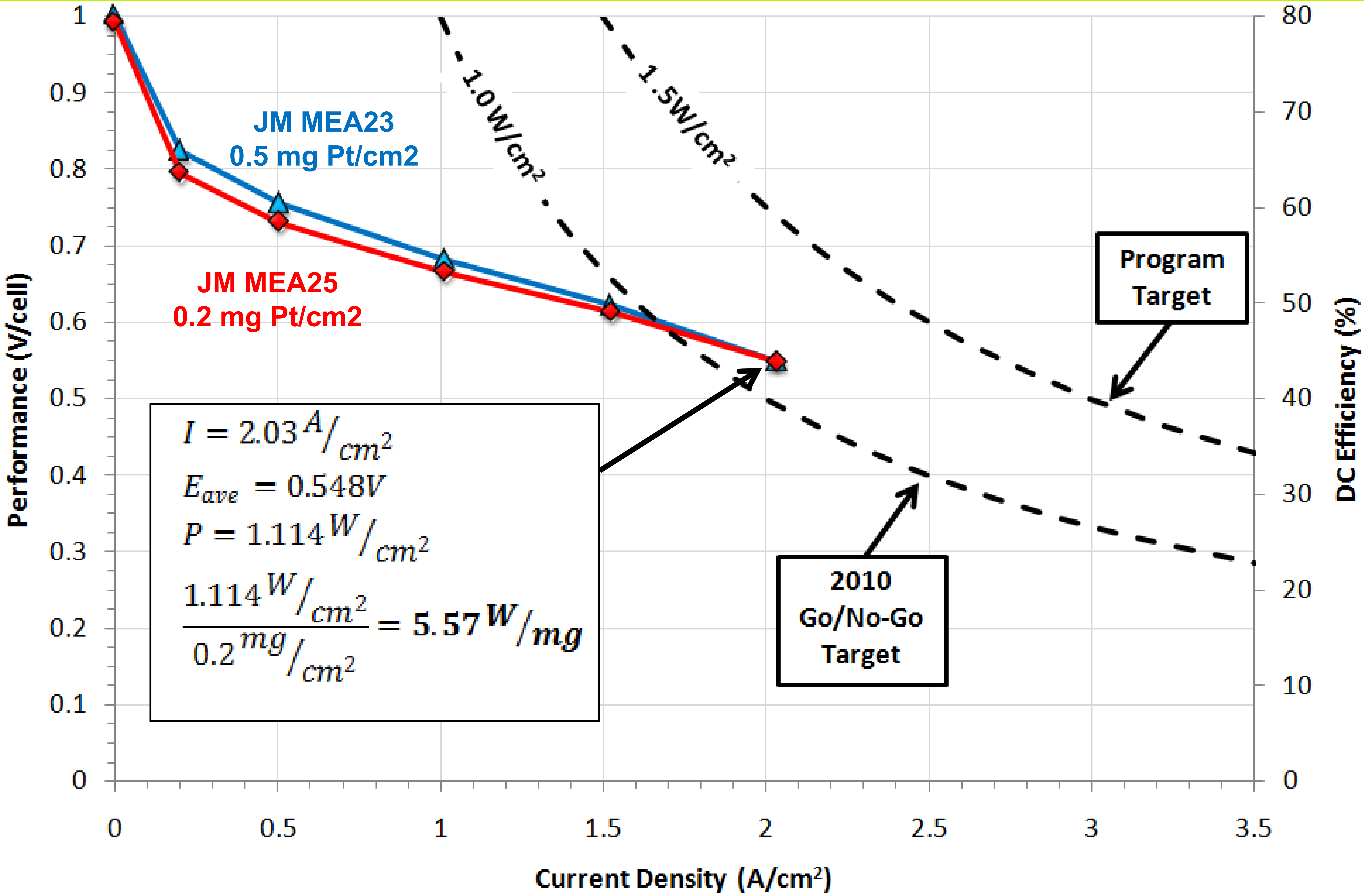
Materials Roadmap

Material development aimed at reducing Pt loading and optimizing performance at high current densities is key to the success of the program



Materials Development Status

The program officially passed the Go/No-Go criteria by demonstrating 1.11 W/cm2 on a 4-cell full format Orion stack.



T_{cell}= 60 °C, An 50% RH, Ca 0% RH, Press ~1.1 to 1.8 bara
MEA23 : JM MEA23, 0.1 mg Pt/cm² An, 0.4 mg Pt/cm² Ca GDL: SGL 25BC
MEA25 : JM MEA25, 0.05 mg Pt/cm² An, 0.15 mg Pt/cm² Ca GDL: SGL 25BC

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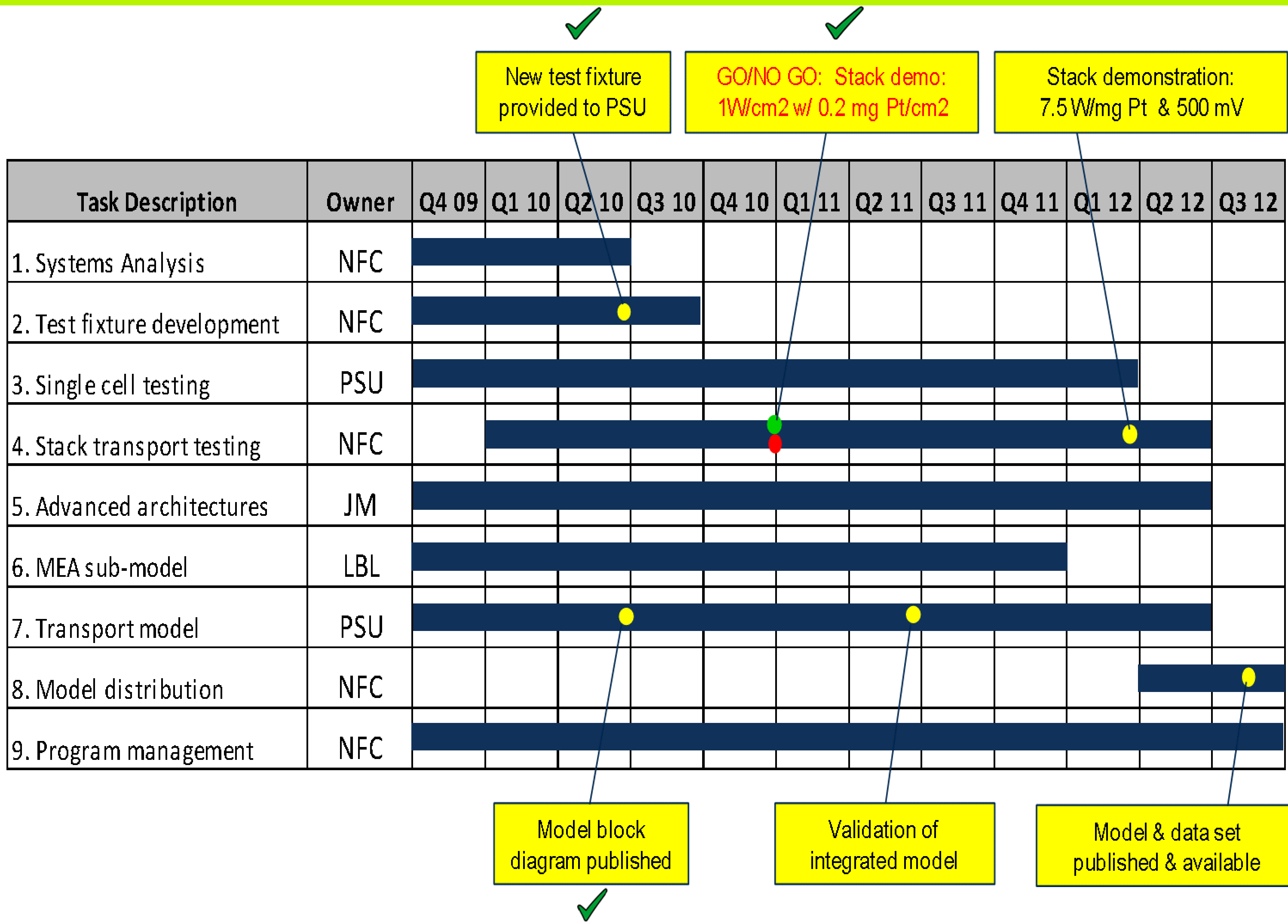
JM Johnson Matthey Fuel Cells — the power within

Plan and Milestones - Approach

The program is on schedule and the Go/No-Go milestone has been met



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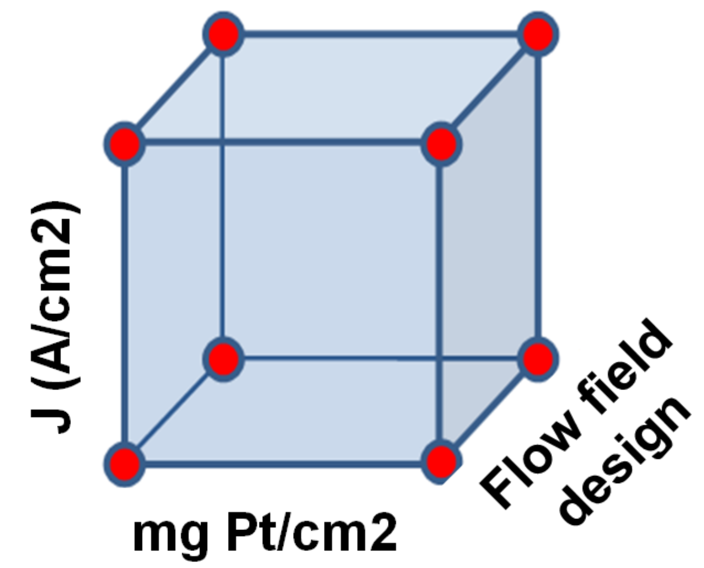
Future Work

Single cell testing

- Test new MEAs to support ongoing materials development
- Perform parametric studies to support model tuning and validation

Model development

- Tune and validate model for:
    - Water balance
    - Current distribution
    - Open Flowfield & Channel/Land architectures



Material development

- MEAs with reduced EW Ionomer in the electrode will be tested in 2011
- MEAs with new electrode structures will be tested in 2011
- MEAs with graded Pt loadings will be tested in 2011

Summary

- The AURORA program plans to achieve DOE cost targets by using a combination of high current density with low Pt loadings.
  - 7.5 W/mgPt => $15/kW
- A model capable of predicting high current density operation in different architectures is the central deliverable of the program.
  - Initial validation and verification are complete
  - Multi-phase physics and agglomerate electrode model are implemented
- Material development aimed at reducing Pt loading and optimizing performance at high current densities is key to the success of the program.
  - Go/No-Go Milestone Passed with stack demonstration of > 5 W/mgPt
- Tests on single cell and full active area stacks will be used to screen new materials, define inputs to the model and validate it.
  - The open flowfield design has demonstrated significant transport advantages
  - Testing of channel/land architecture provides relevant data to the FC community

Technical Back-Up Slides

Test Conditions

Orion Automotive Conditions

Current Density	Current	Anode Stoich.	Anode Flow	Anode Inlet Pressure	Anode Dewpoint Temp.	Cathode Stoich.	Cathode Flow	Cathode Dewpoint Temp.	Cathode **Inlet** Pressure	Coolant Flow	Cooing Inlet Temp.
(A/cm2)	(A)	(#)	(SLPM)	(mbar)	(°C)	(#)	(SLPM)	(°C)	(mbar)	(LPM)	(°C)
0.20	50.00	2.15	3.00	300.00	46.00	**2.00**	6.67	DRY	300.00	1.50	60.00
0.50	125.00	2.00	6.97	300.00	46.00	**2.00**	16.67	DRY	300.00	1.50	60.00
1.00	250.00	2.00	13.94	530.00	46.00	1.80	30.00	DRY	530.00	2.00	60.00
1.50	375.00	2.00	20.91	750.00	46.00	1.90	47.50	DRY	750.00	3.00	60.00
2.00	500.00	2.00	27.88	800.00	46.00	2.00	66.67	DRY	800.00	4.00	60.00

50 cm^2 Conditions

Current Density	Current	Anode Stoich.	Anode Flow	Anode Inlet Pressure	Anode Dewpoint Temp.	Cathode Stoich.	Cathode Flow	Cathode Dewpoint Temp.	Cathode **Inlet** Pressure	Coolant Flow	Cooing Inlet Temp.
(A/cm2)	(A)	(#)	(SLPM)	(mbar)	(°C)	(#)	(SLPM)	(°C)	(mbar)	(LPM)	(°C)
0.13	6.25	2.00	0.09	106.75	46.00	1.60	0.17	DRY	106.75	64.00	60.00
0.25	12.50	2.00	0.18	166.75	46.00	1.60	0.33	DRY	166.75	64.00	60.00
0.50	25.00	2.00	0.35	276.75	46.00	1.70	0.71	DRY	276.75	64.00	60.00
1.00	50.00	2.00	0.70	506.75	46.00	1.80	1.50	DRY	506.75	128.00	60.00
1.50	75.00	2.00	1.05	736.75	46.00	1.90	2.38	DRY	736.75	200.00	60.00
2.00	100.00	2.00	1.40	786.75	46.00	2.00	3.33	DRY	786.75	320.00	60.00
2.50	125.00	2.00	1.75	786.75	46.00	2.00	4.17	DRY	786.75	400.00	60.00
3.00	150.00	2.00	2.10	786.75	46.00	2.00	5.00	DRY	786.75	480.00	60.00

Backup slides about agglomerate model

Assumptions:

- isothermal, equipotential agglomerate.
- 1st order reaction of ORR

Transfer current density J_{gen} [A/m^3]

$$J_{gen} = 4F\left(\frac{C_{O_2}}{H/RT}\right)^{\gamma_c}\left[\frac{1}{(1-\varepsilon_0)E_r k_c} + \frac{\delta}{a_{agg}D_{O_2,Nafion}}\cdot\frac{r_{agg}+\delta}{r_{agg}}\right]^{-1}(1-s)$$

Effectiveness factor E_r

$$E_r = \frac{1}{\phi_L}\left(\frac{1}{\tanh(3\phi_L)} - \frac{1}{3\phi_L}\right)$$

Thiele modulus

$$\phi_L = \frac{r_{agg}}{3}\sqrt{\frac{k_c}{D_{O_2,agg}^{eff}}}$$

Reaction rate constant k_c [s^{-1}]

$$k_c = \frac{a i_{0,c}^{ref}}{4FC_{O_2,ref}^{\gamma_c}}\exp\left(-\frac{\alpha_c F}{R_u T}\eta\right)$$