

Computer-Aided Optimization of Macroscopic Design Factors for Lithium-Ion Cell Performance and Life



*217th Electrochemical
Society Meeting
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April 29, 2010*

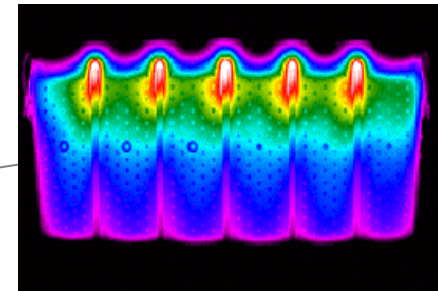
Kandler Smith,
Gi-Heon Kim,
Ahmad Pesaran

NREL/PR-5400-47947

Motivation for Battery CAE

Cell/battery **development process** of testing new materials in multiple cell sizes, in multiple pack designs, and over many months is extremely **time consuming, expensive, and ad hoc.**

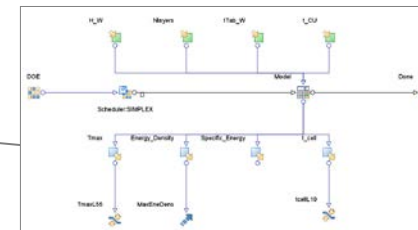
- Large cells/batteries suffer from heat, current, stress issues not present in small configurations



Thermal Image of Gen I Toyota Prius Module

Computer-aided engineering (CAE) processes offer methodology to **shorten design cycle** and optimize batteries for **thermal uniformity, safety, long life, low cost.**

- Proven examples from automotive and aerospace
- Robust design, 6-sigma, design optimization,...



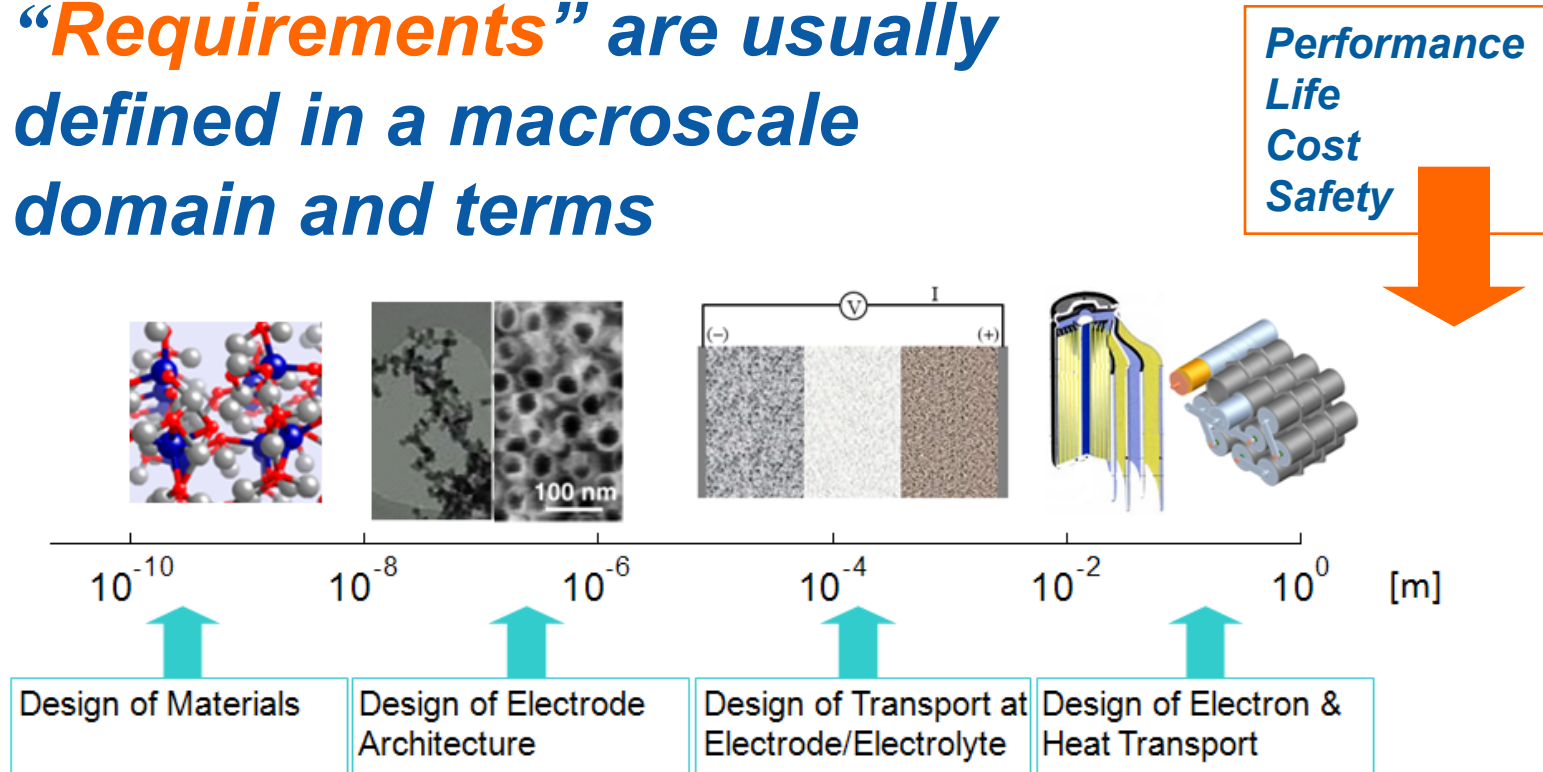
Process Integration, Design & Optimization (PIDO) Software

Requirements for large battery CAE:

- Efficient mathematical models (desktop PC)
- Capture correct **physics** and **3D geometry**

Multi-Scale Physics in Li-Ion Battery

“Requirements” are usually defined in a macroscale domain and terms

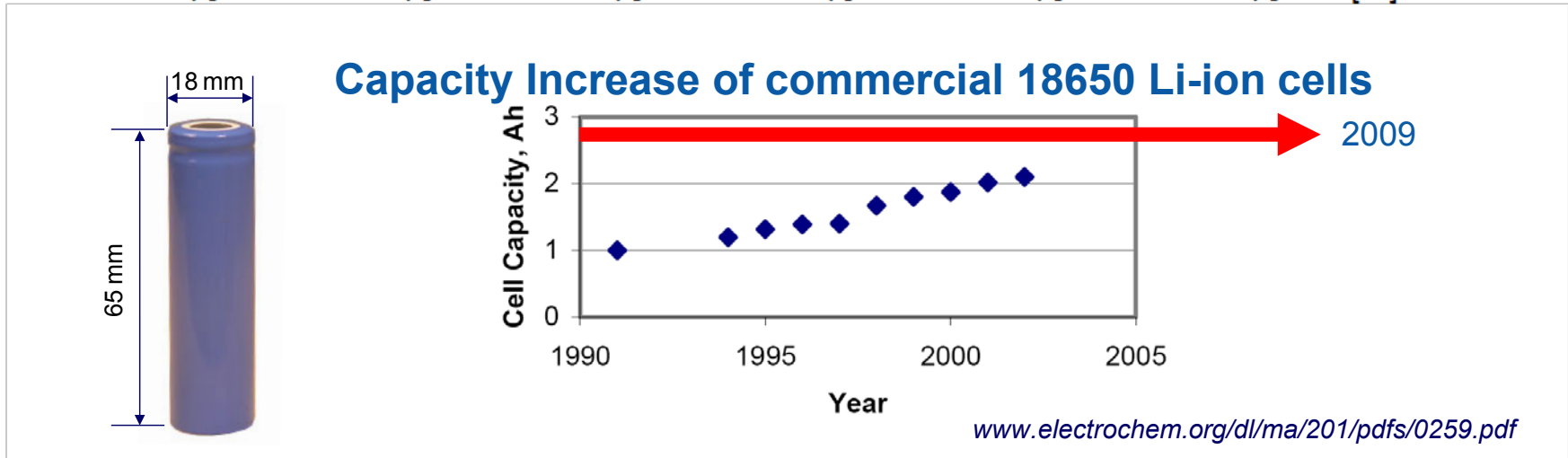
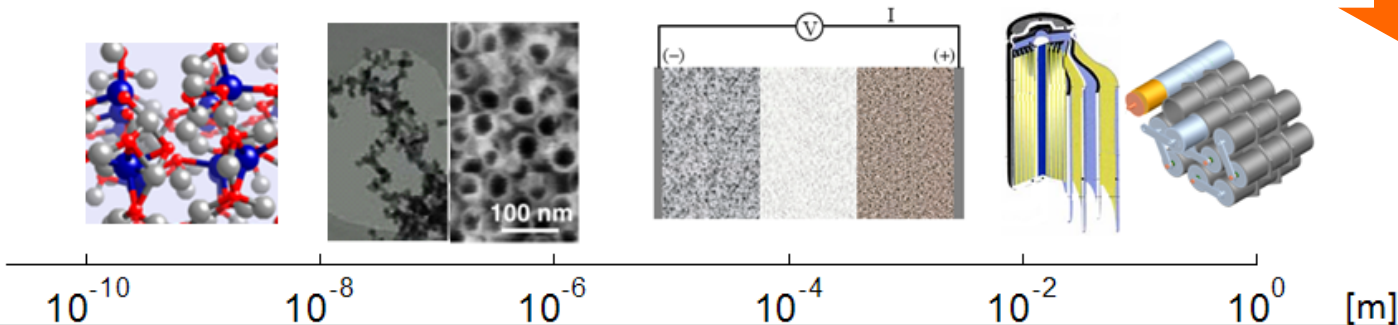


- Wide range of length and time scale physics
- Design improvements required at different scales
- Need for better understanding of interaction among different scale physics

Multi-Scale Physics in Li-Ion Battery

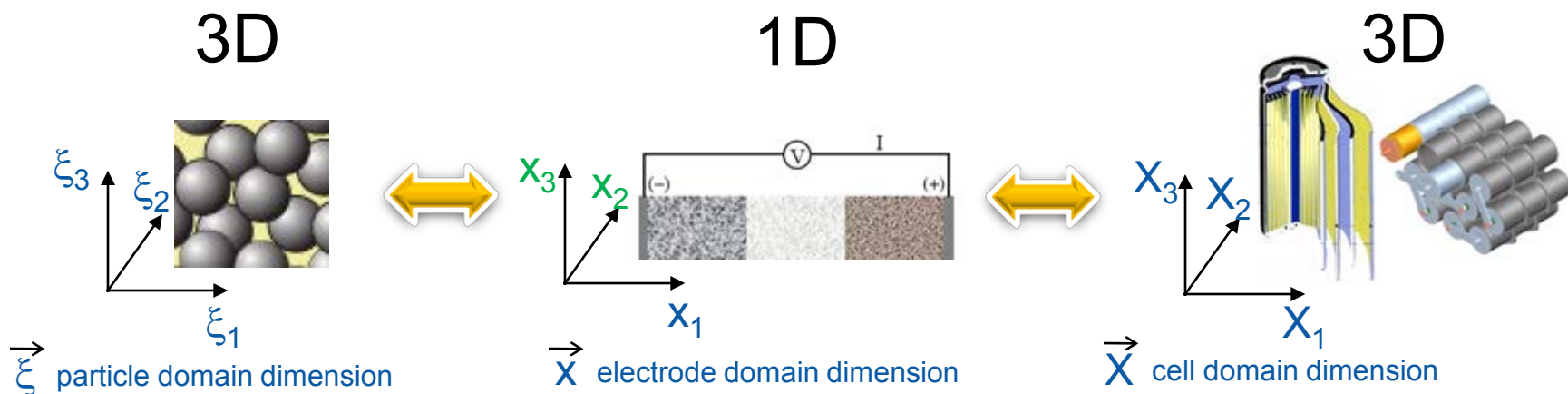
“Requirements” are usually defined in a macroscale domain and terms

Performance
Life
Cost
Safety

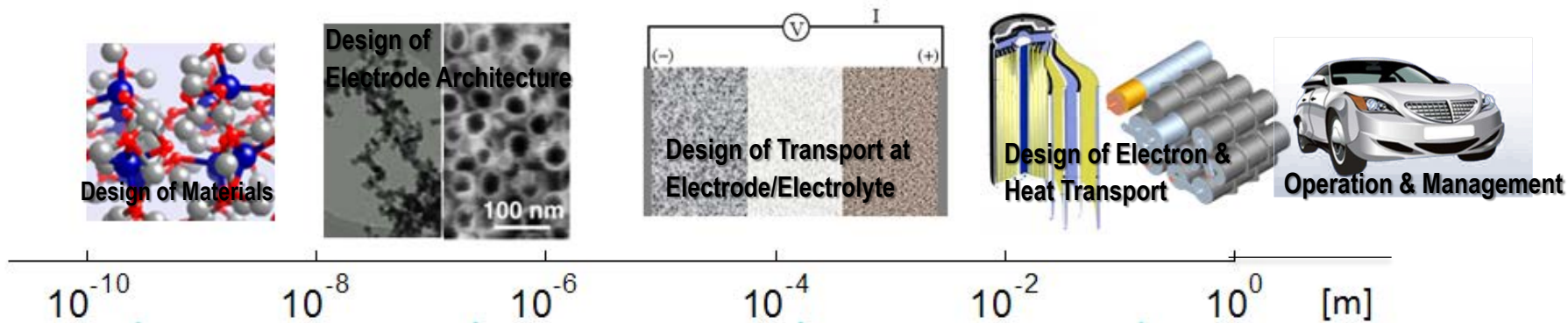


NREL's Multi-Scale Multi-Dimensional Model Approach

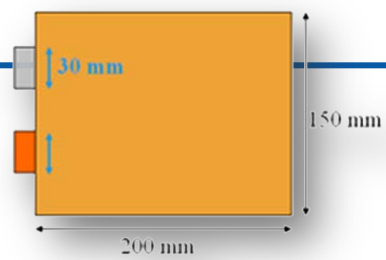
Efficient representation of 3D electrochemical/thermal physics



NREL
MSMD- μ MSMD-c



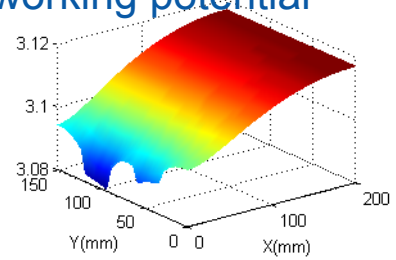
Importance of Multi-Physics Interaction



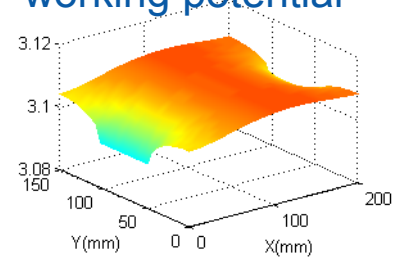
Comparison of two 40 Ah flat cell designs
2 min 5C discharge



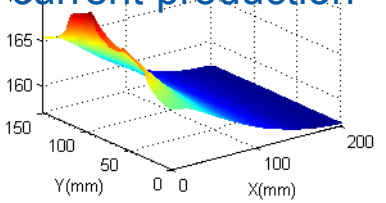
working potential



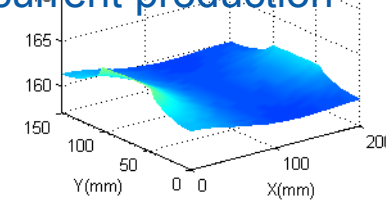
working potential



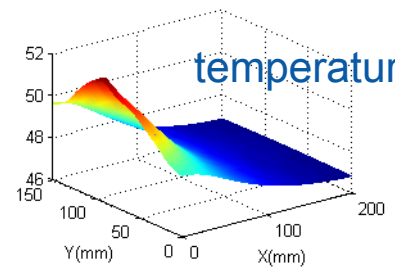
electrochemical current production



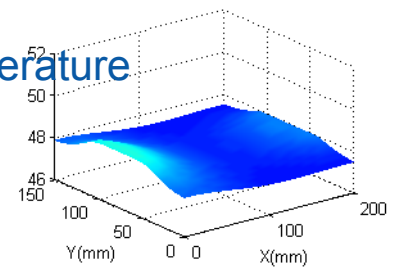
electrochemical current production



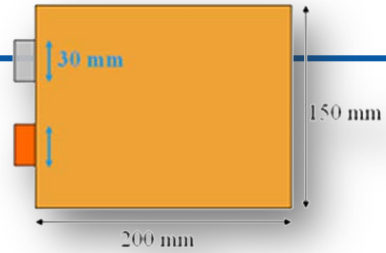
temperature



temperature



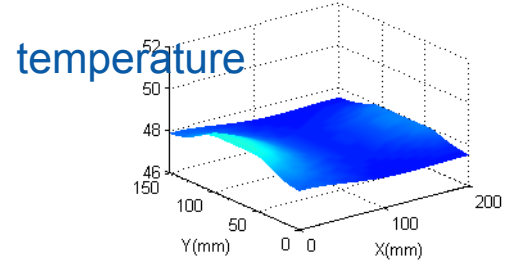
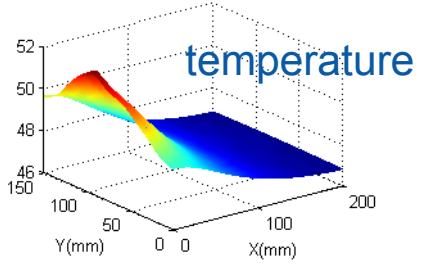
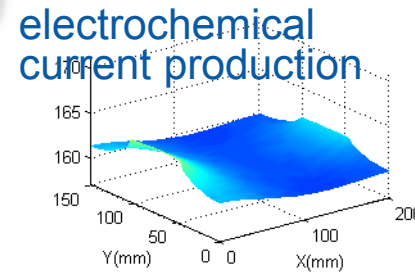
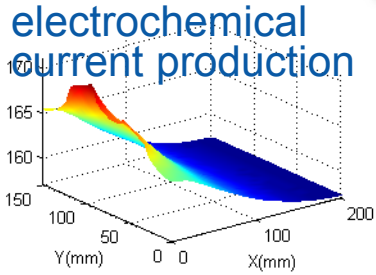
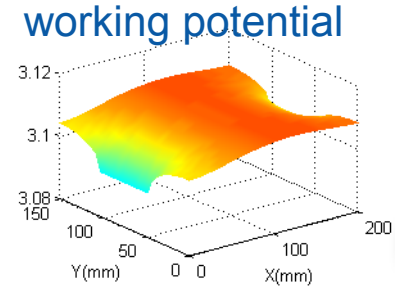
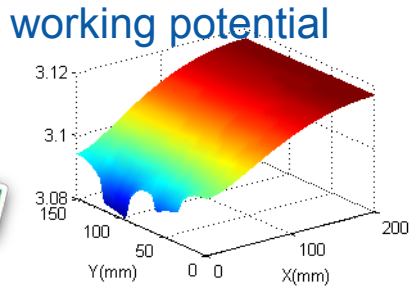
Importance of Multi-Physics Interaction



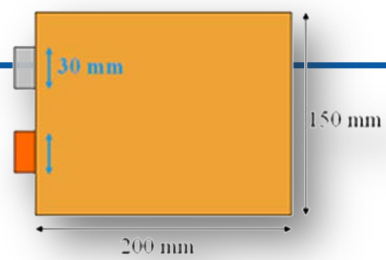
Comparison of two 40 Ah flat cell designs
2 min 5C discharge



- Larger over-potential promotes faster discharge reaction
- Converging current causes higher potential drop along the collectors



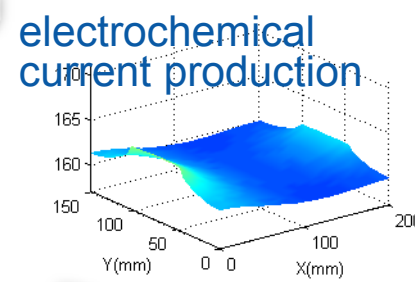
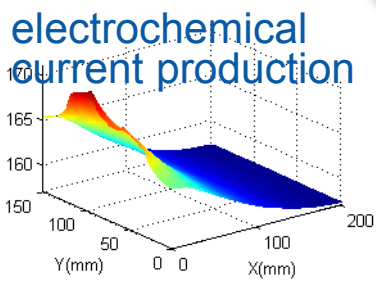
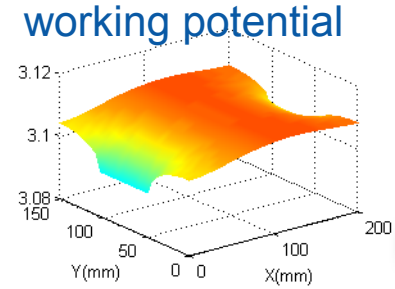
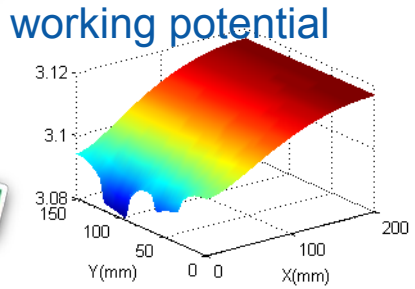
Importance of Multi-Physics Interaction



Comparison of two 40 Ah flat cell designs
2 min 5C discharge



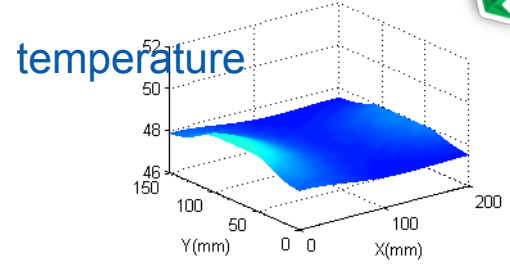
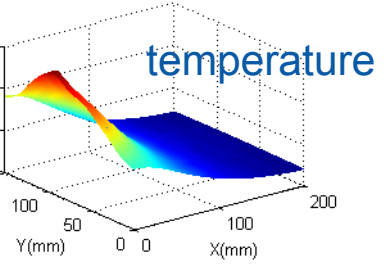
- Larger over-potential promotes faster discharge reaction
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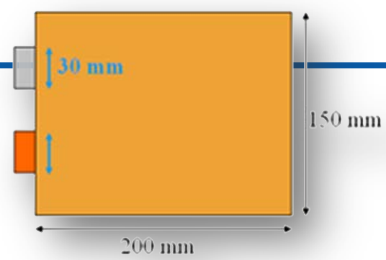
SOC

SOC

- High temperature promotes faster electrochemical reaction
- Higher localized reaction causes more heat generation



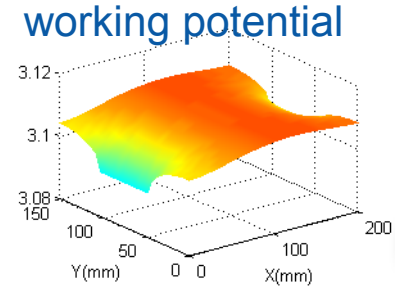
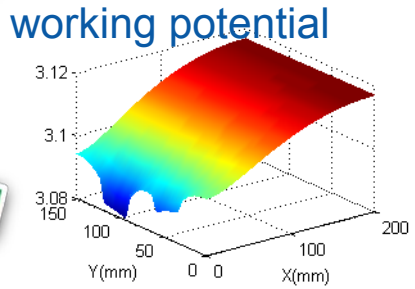
Importance of Multi-Physics Interaction



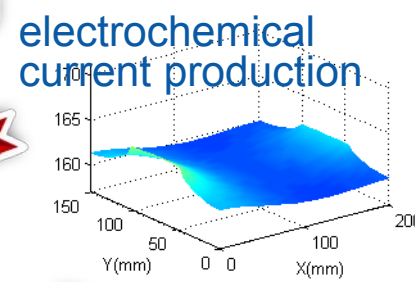
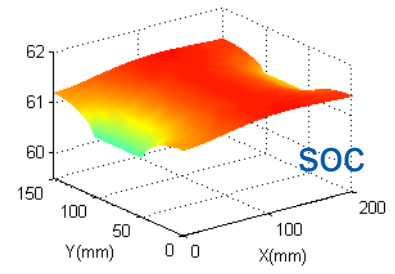
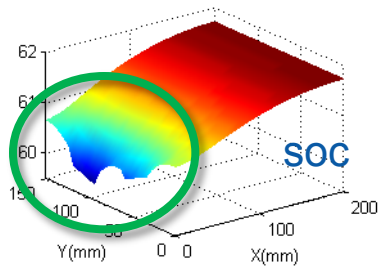
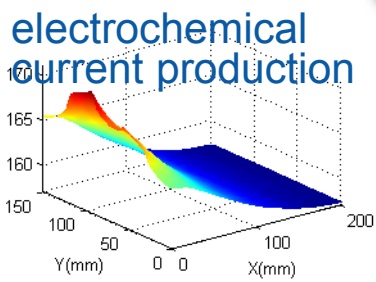
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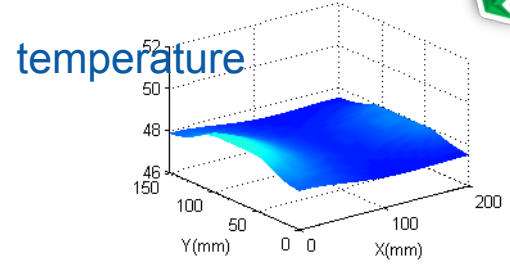
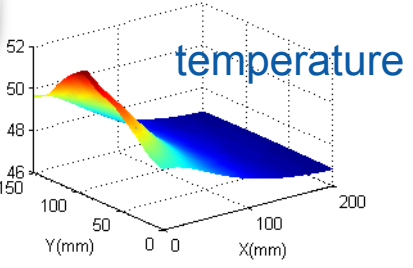
- Larger over-potential promotes faster discharge reaction
- Converging current causes higher potential drop along the collectors



This cell is cycled more uniformly, can therefore use less active material (\$) and is expected to have longer life.



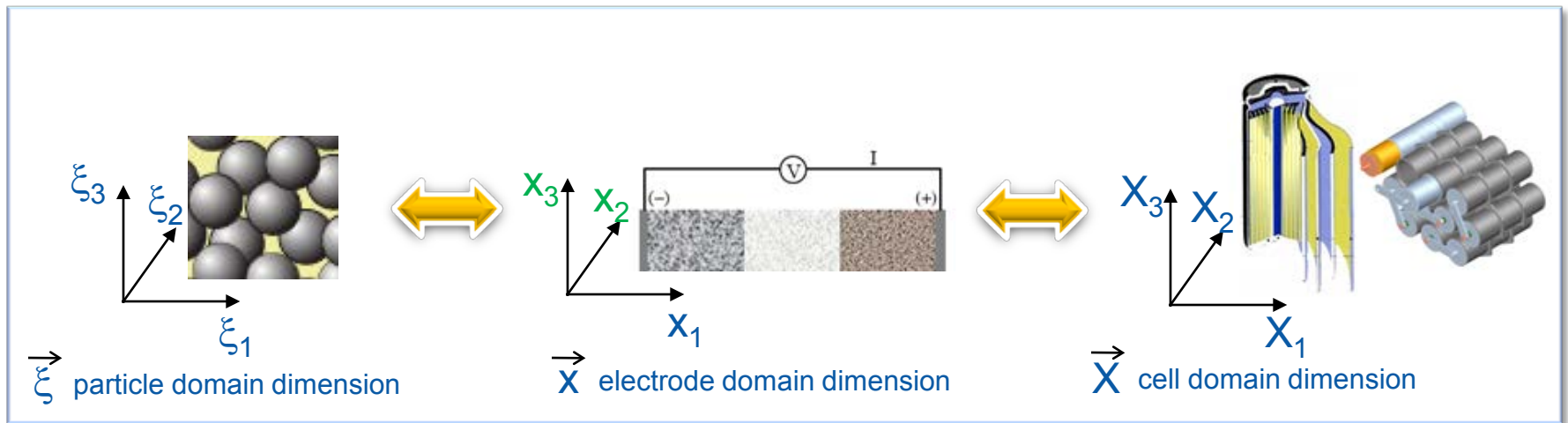
- High temperature promotes faster electrochemical reaction
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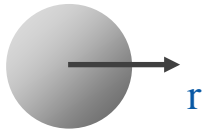
Present Study

- Problem definition
 - Model description
 - Macroscopic design parameters chosen for optimization (fixed electrode design)
 - Design evaluation criteria
 - Optimization procedure (numerical DoE)
- Results
 - Response surface
 - Optimal designs
- Conclusions

Model Realization for 20 Ah Stacked Prismatic Cell



1D

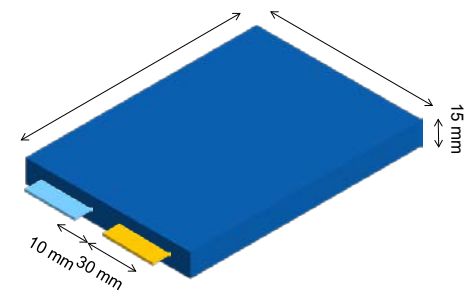


1D

SVM



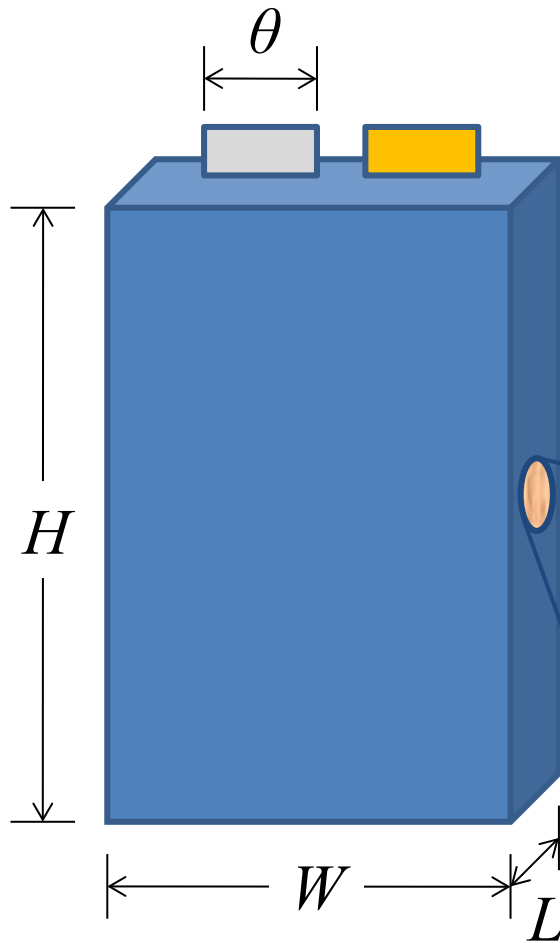
2D



- ✓ *Reduced order model derived from governing equations of Doyle, Fuller, Newman, 1993.*
- ✓ *Chose parameters representative of NCA/graphite chemistry*

- ✓ *Stacked prismatic design*
- ✓ *Various form factors*
- ✓ *Tabs on same side*
- ✓ *20 Ah*
- ✓ *PHEV10 application*

Macroscopic Design Parameters Chosen for Optimization

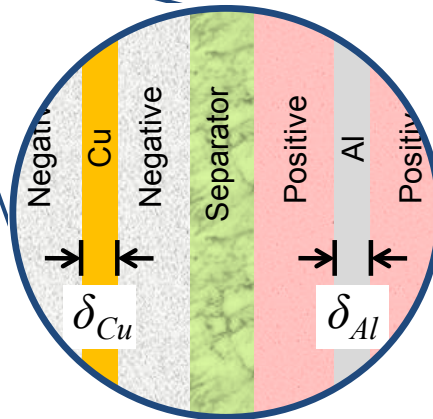


Aspect ratio, H/W

Tab width, θ/W

Electrode layers, N

Foil thickness, δ_{Cu}



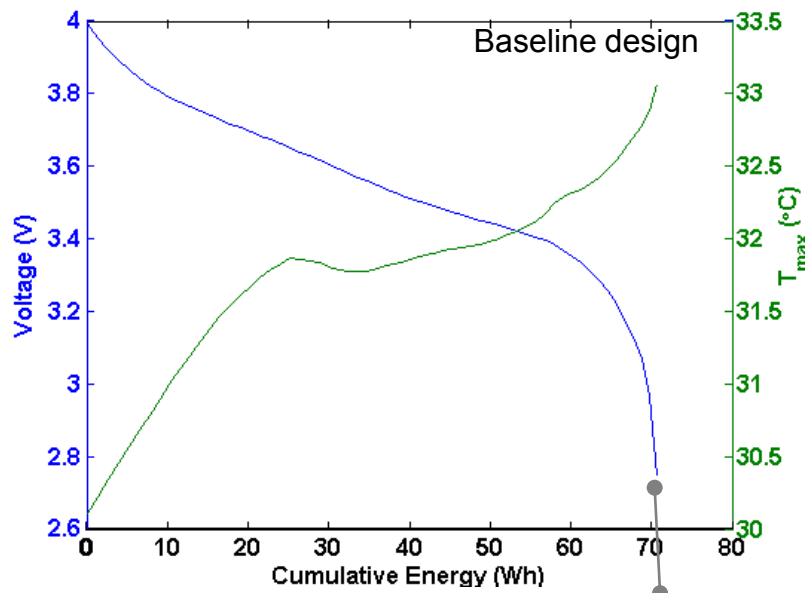
Other design parameters fixed:

- $\delta_{Al} = 1.6 \times \delta_{Cu}$
 - 20 Ah capacity
 - Electrode loadings
 - Electrode thicknesses
- (Typical tradeoff between power & energy do not arise in this study)

Cell Design Evaluation Criteria

Energy at 2C rate

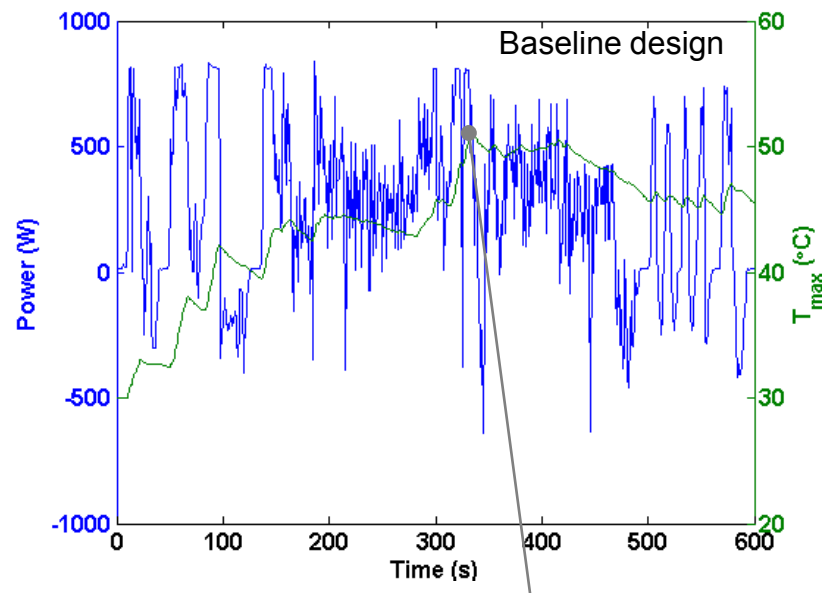
- Energy density (Wh/L) evaluated at module level (includes 5mm external tab height + 3 mm cooling channel between cells)



71 Wh

Maximum temperature during driving cycle

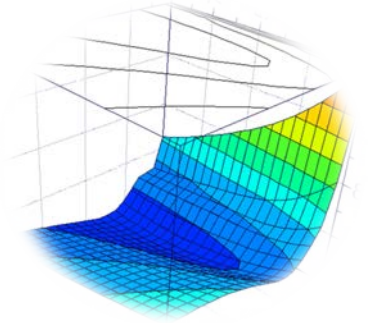
- 10-mile PHEV charge depletion cycle



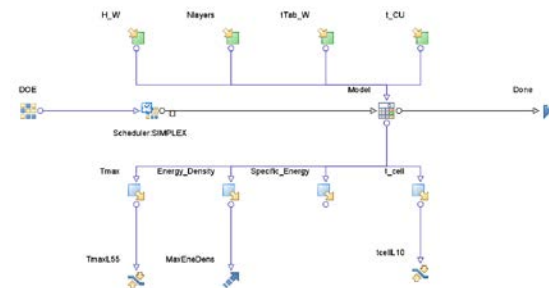
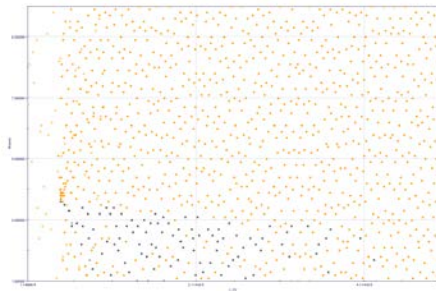
51°C peak

Optimization Process Steps - 1

1. Use Design Of Experiments to generate 50 design points
2. Execute NREL's 3D Electrochemical-Thermal Multi-Physics Model for all 50 DOE points
3. From the 50 DOE points use an advanced response surface technique (Radial based Functions) to generate 4 response surface functions:
 - a) T_{max} (Nlayers, t_{CU} , H_W , t_{Tab_W})
 - b) Energy_Density (Nlayers, t_{CU} , H_W , t_{Tab_W})
 - c) Specific_Energy (Nlayers, t_{CU} , H_W , t_{Tab_W})
 - d) Cell Thickness (Nlayers, t_{CU} , H_W , t_{Tab_W})



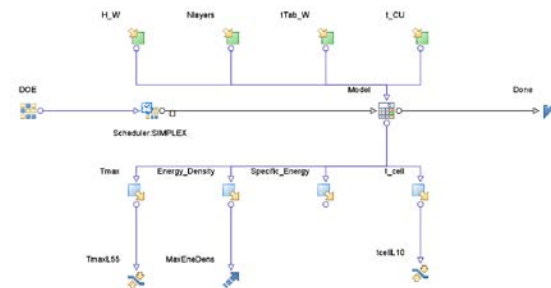
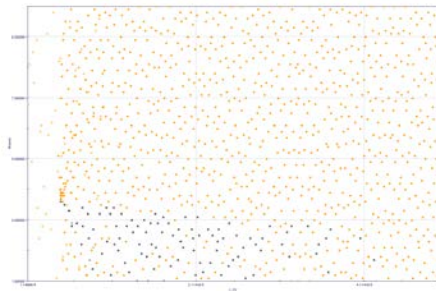
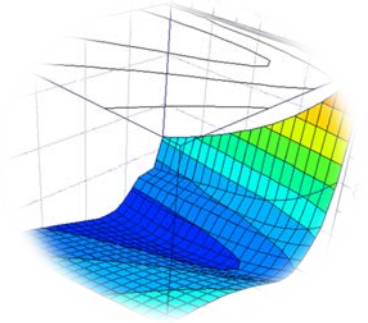
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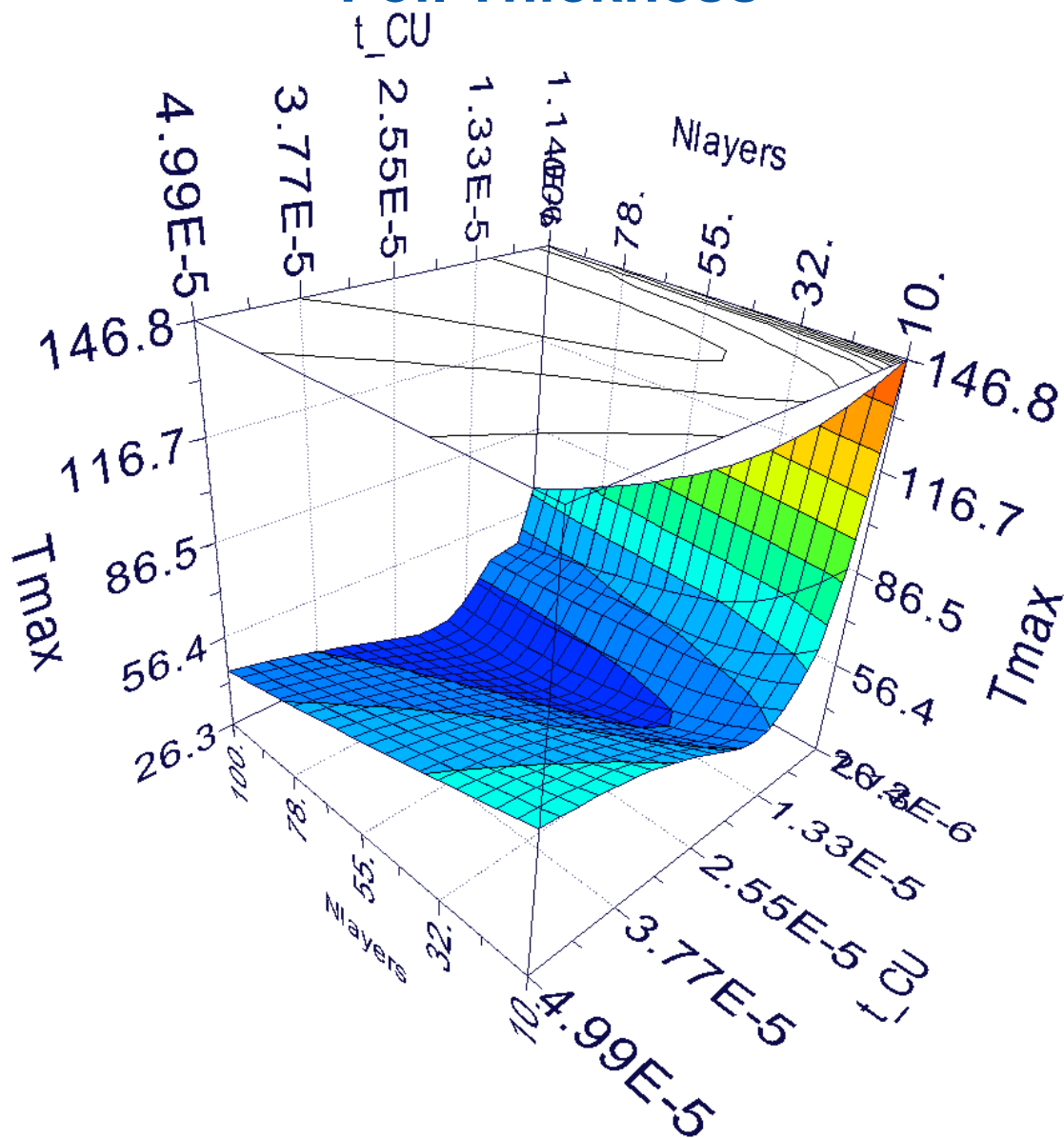
Optimization Process Steps - 2

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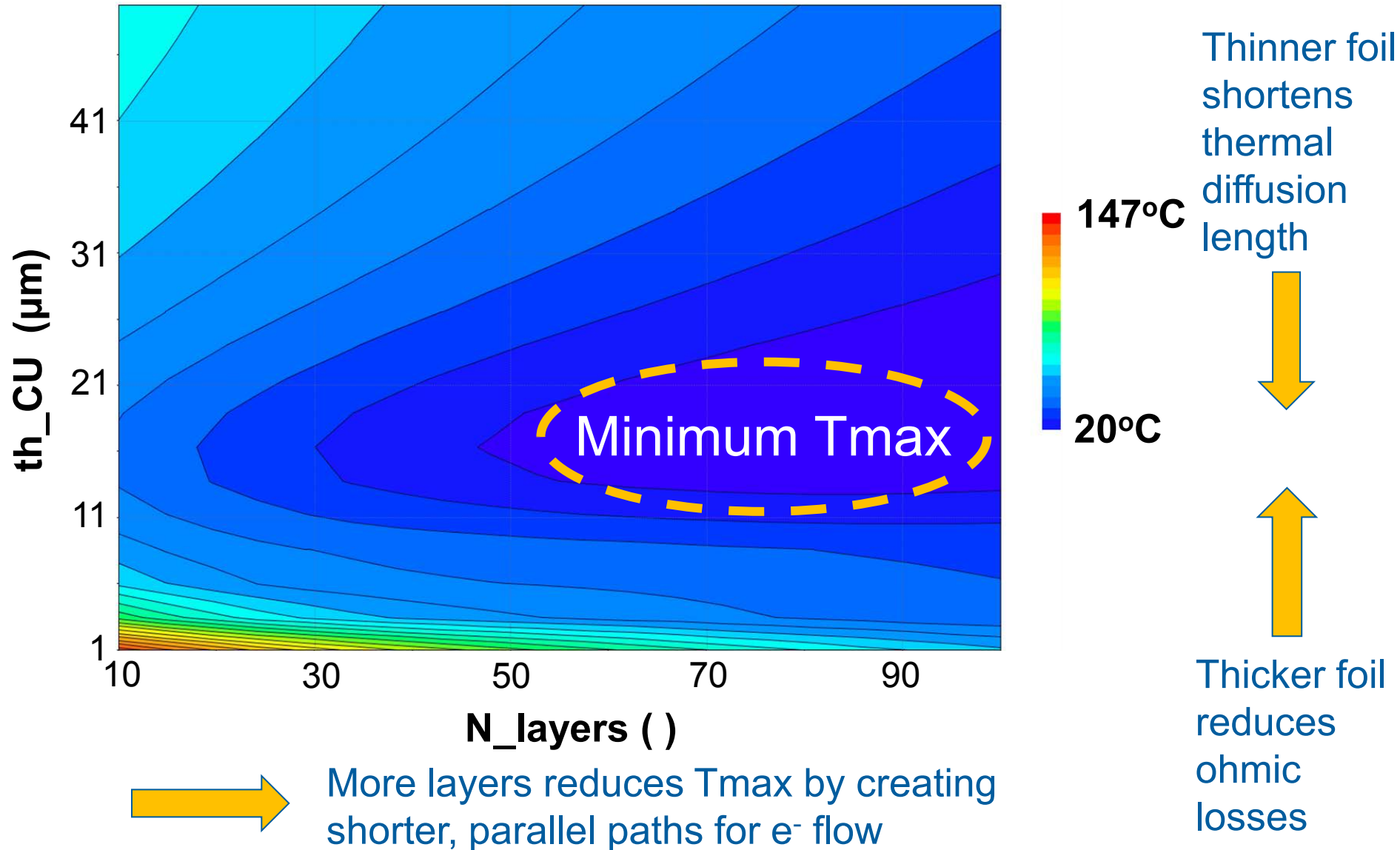
4. Generate 1000 more DOE points using a simple sampling technique (Sobol)
5. Run the 1000 DOE points through the 4 response functions to generate 1000 more data points
6. Select the best of the 1050 design points and use it as starting point for an optimization algorithm
7. The optimizer tries to maximize the energy density with two constraints a) $T_{max} < 55\text{ C}$ and b) $L < 16\text{ mm}$
8. Identify the top two optimum points



Tmax Response Surface versus Number of Layers & Cu Foil Thickness

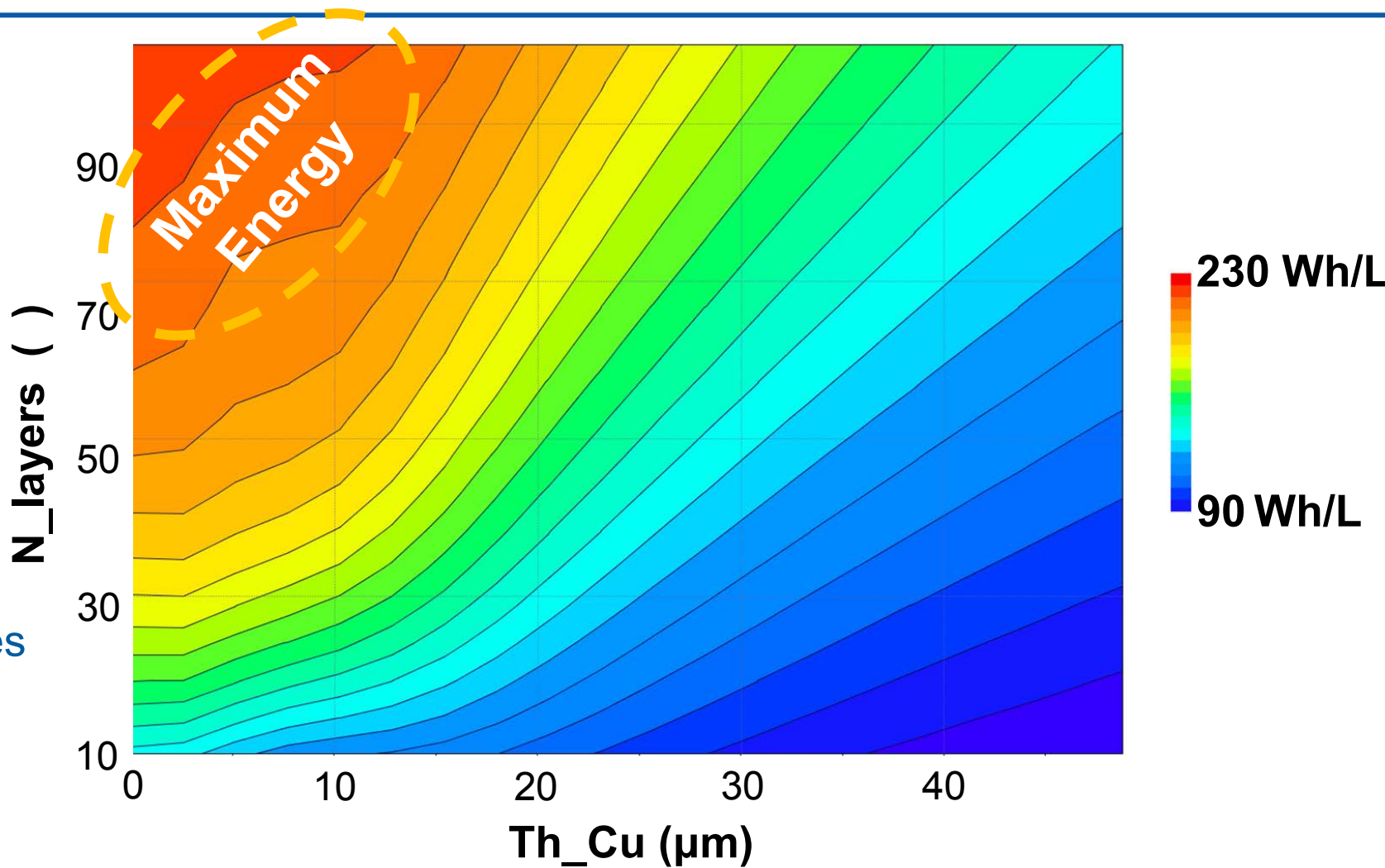


Tmax versus Number of Layers & Cu Foil Thickness



Energy Density* versus Number of Layers & Cu Foil Thickness

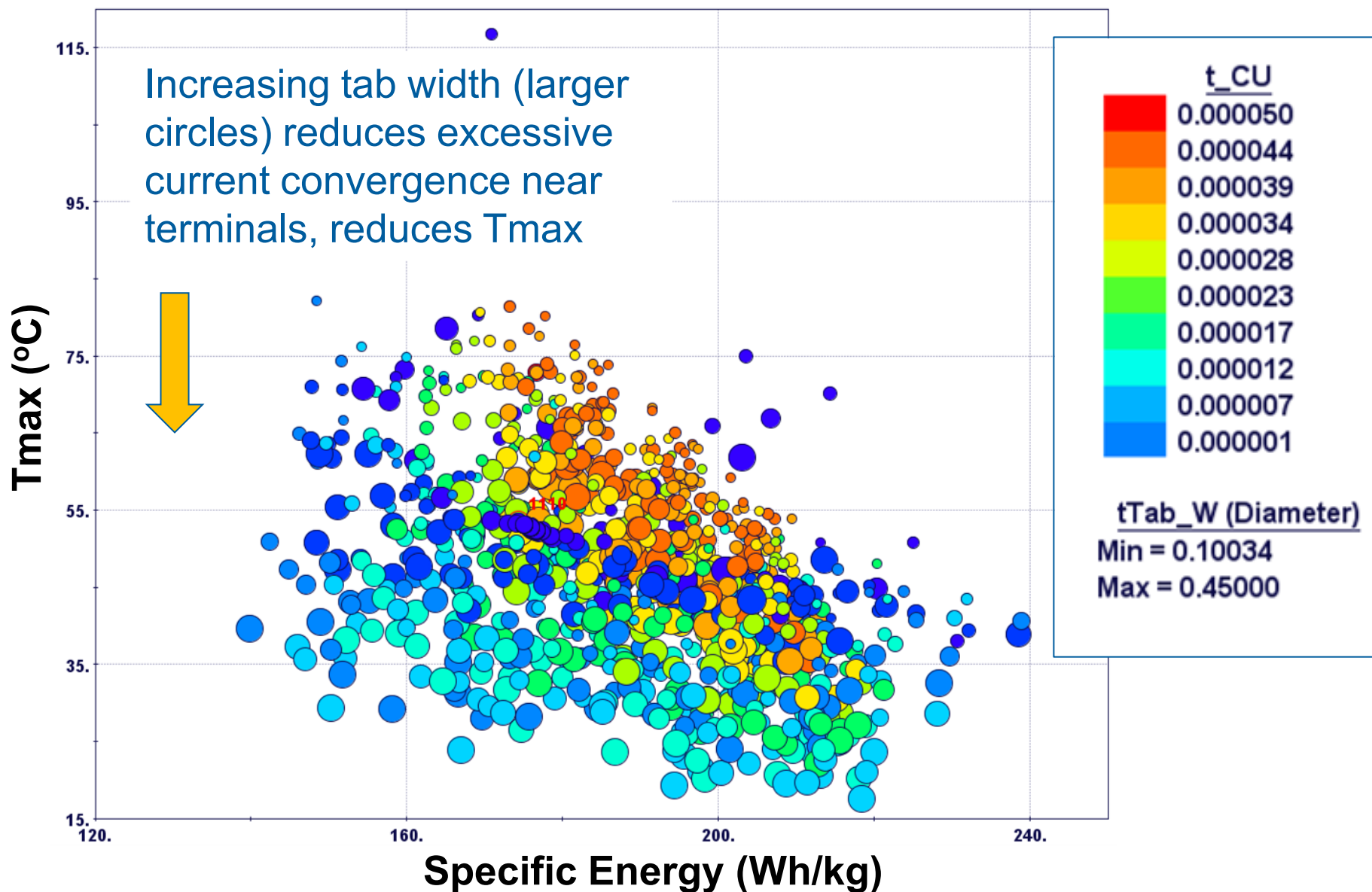
↑
More parallel layers reduces losses, maximizes useable energy



Less foil reduces volume, mass of inert components

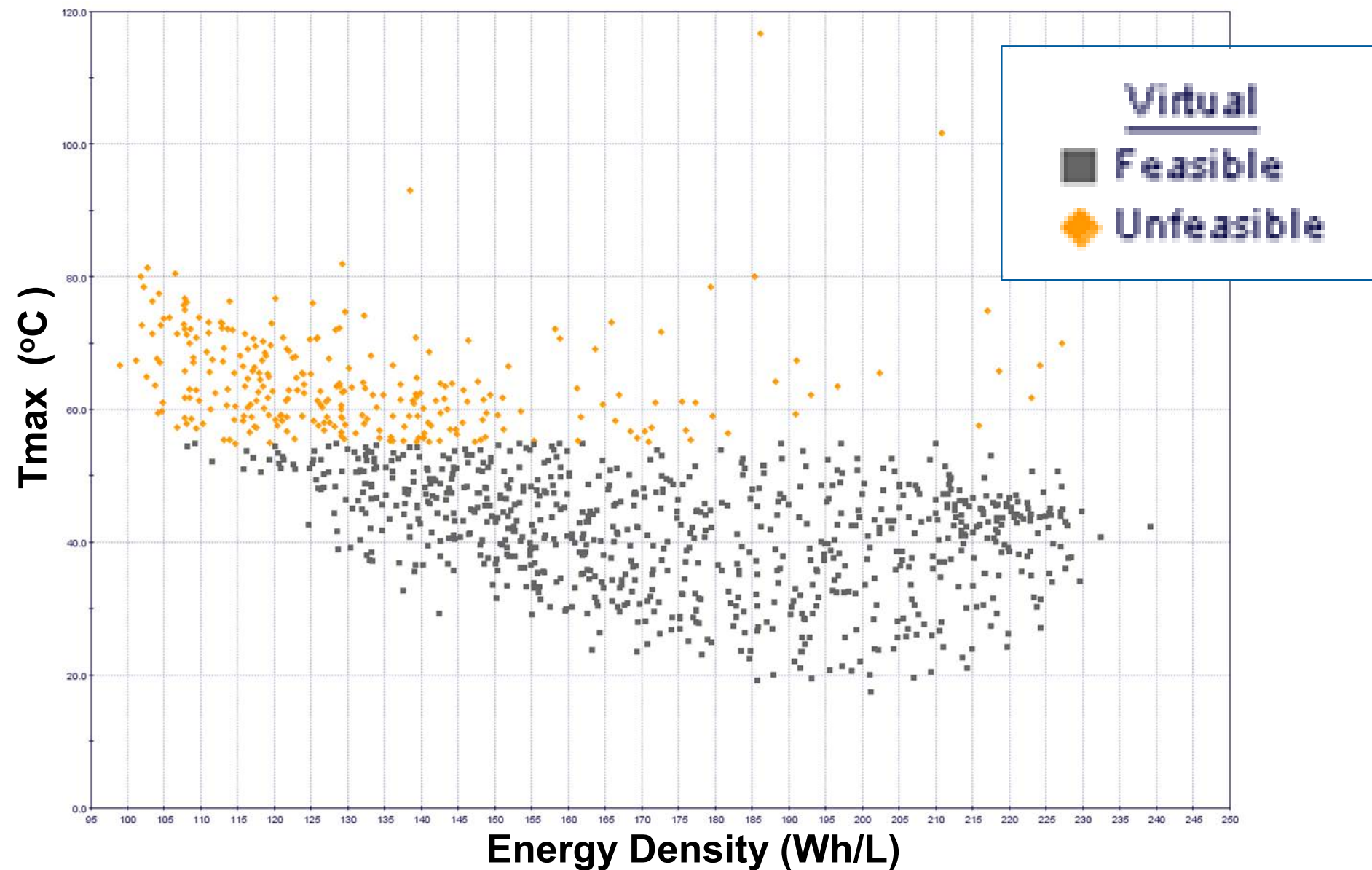
*2C rate, module level Wh/L

Scatter Plot of Tmax versus Specific Energy for various values of Cu thickness and tab width ratio



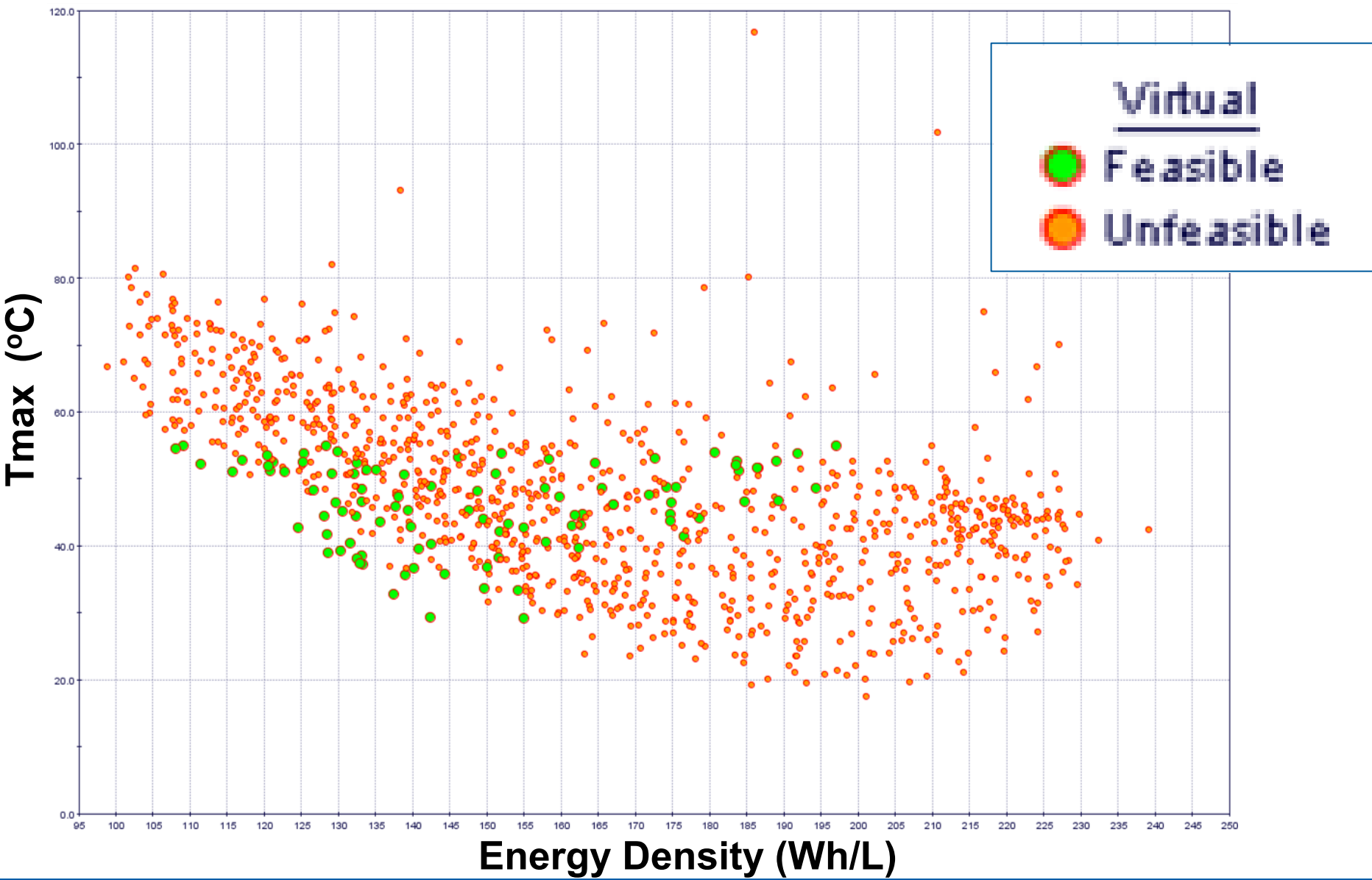
Scatter Plot of Tmax versus Energy Density

Feasible points with Tmax < 55°C

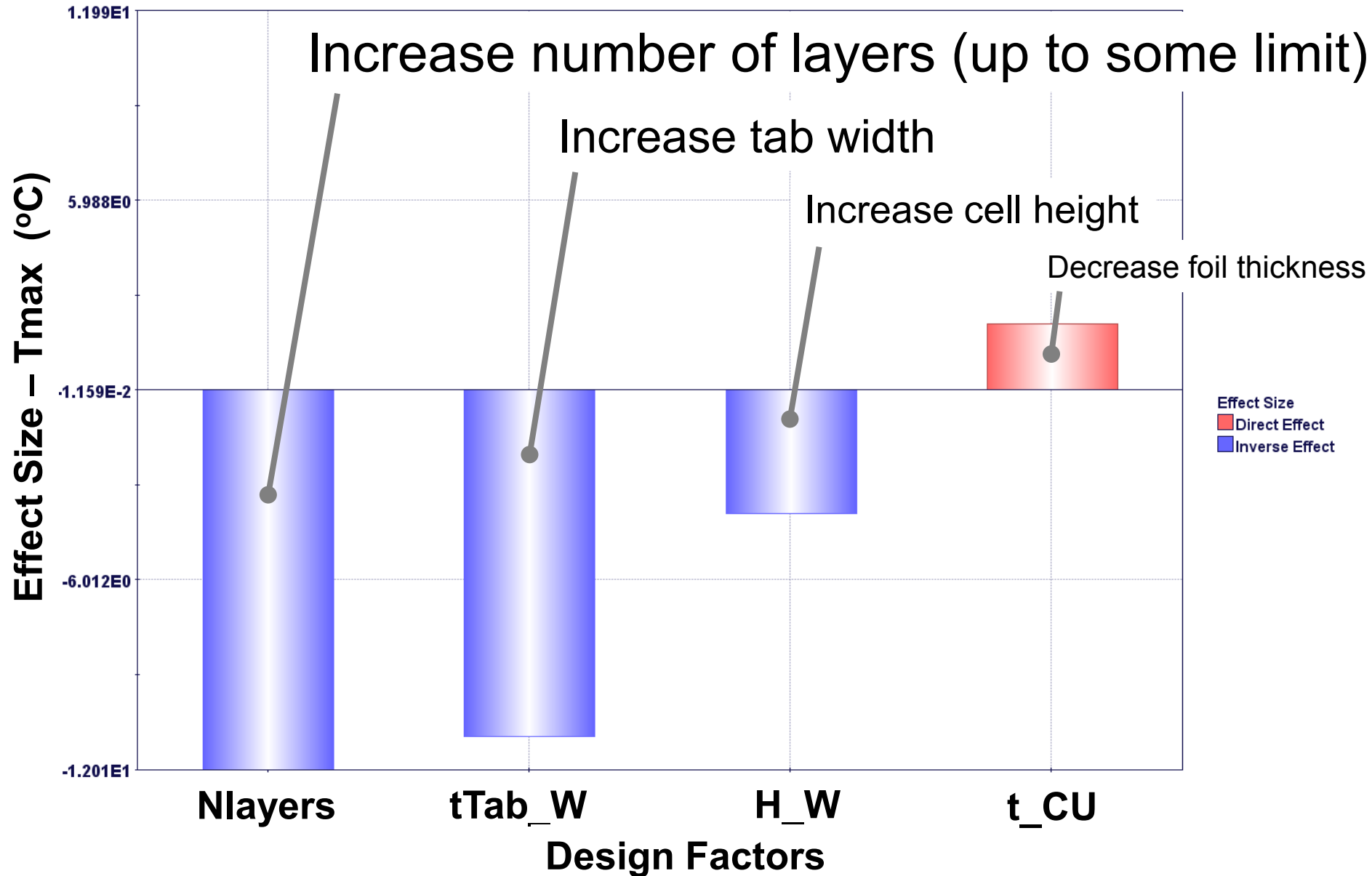


Scatter Plot of Tmax versus Energy Density

Feasible points with Tmax < 55°C and Cell thickness < 16 mm

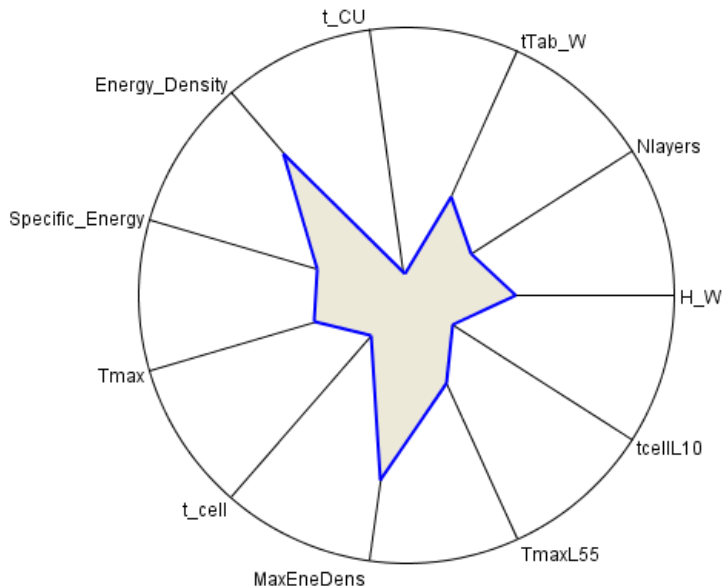


Effect of Design Variables on Tmax (minimize)



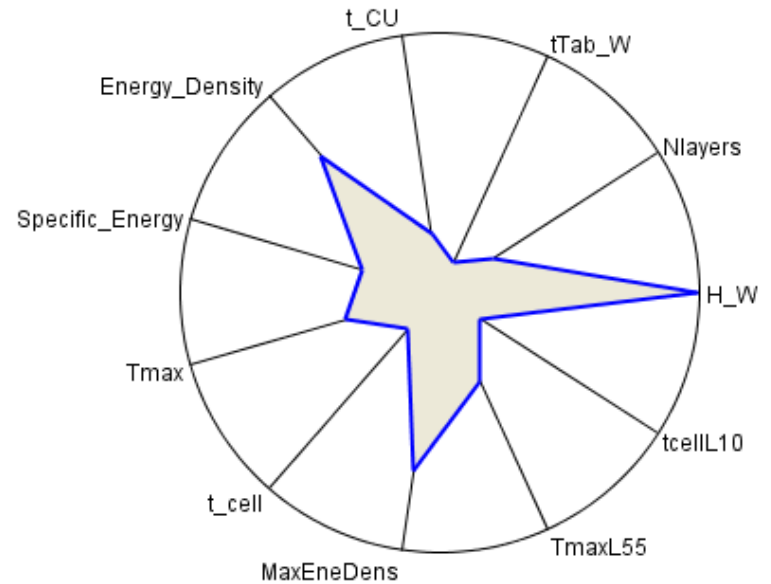
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Type	Virtual Design	
Input Variables		
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Nlayers		3.600E1
tTab_W		2.422E-1
t_CU		5.000E-6
Output Variables		
Energy_Density		1.973E2
Specific_Energy		1.743E2
Tmax		5.354E1
t_cell		1.098E-2
Objectives		
MaxEneDens		1.9730E2
Constraints		
TmaxL55		5.3542E1
tcellL10		1.0981E-2

Optimum Design Point #1



Design ID	698	
Type	Virtual Design	
Input Variables		
H_W		2.982E0
Nlayers		3.200E1
tTab_W		1.461E-1
t_CU		1.225E-5
Output Variables		
Energy_Density		1.970E2
Specific_Energy		1.708E2
Tmax		5.502E1
t_cell		1.043E-2
Objectives		
MaxEneDens		1.9697E2
Constraints		
TmaxL55		5.5024E1
tcellL10		1.0428E-2

Optimum Design Point #2



Optimal vs. Base Cell Design

	Design Parameters				Simulated Performance	
	N Layers ()	Cu foil thkness (μm)	H (mm)	L (mm)	Energy Density* (Wh/L)	US06 Tmax ($^{\circ}\text{C}$)
Base	19	10	248	6.3	166	50.6
Opt1	36	5	187	16.2	258	43.0
Opt2	32	12.3	191	16.6	261	39.5

More layers

Shorter height



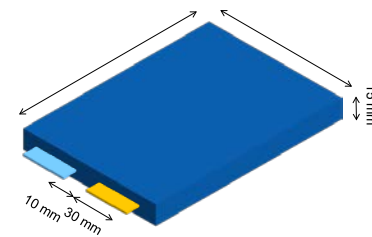
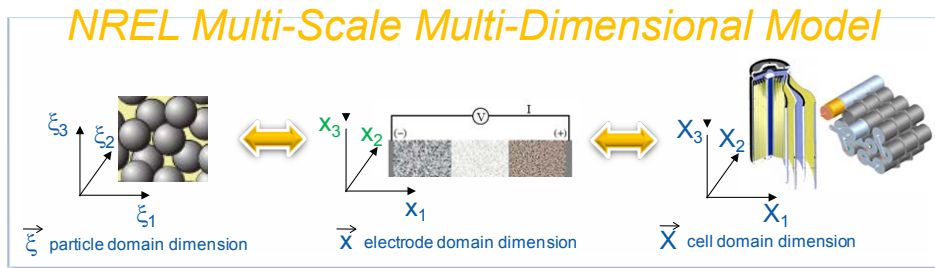
Improved energy density

Peak temperatures reduced 10 $^{\circ}\text{C}$

*module level energy density includes 5mm external tab height & fixed 3mm intercell gap

Conclusions

- Large cell design is challenging problem of competing requirements & objectives
- Robust design CAE methods provide straightforward process for optimization, so long as
 - Objectives & constraints are well-defined
 - Physics and geometry are properly captured
- Compared to baseline design, optimization of macroscopic factors decreases peak temperatures (fewer losses in cell) while increasing useable energy density



Acknowledgements

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U.S. Department of Energy

Thank you