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

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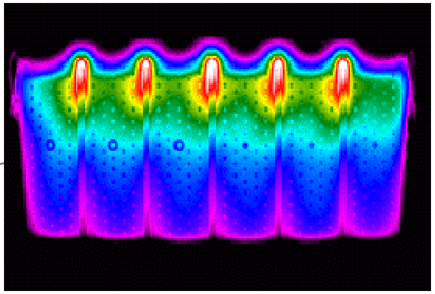
NREL is a national laboratory of the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, operated by the Alliance for Sustainable Energy, LLC.

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.

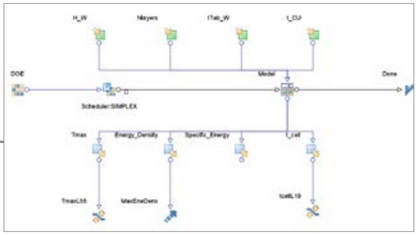
- Large cells/batteries suffer from heat, current, stress issues not present in small configurations



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,…



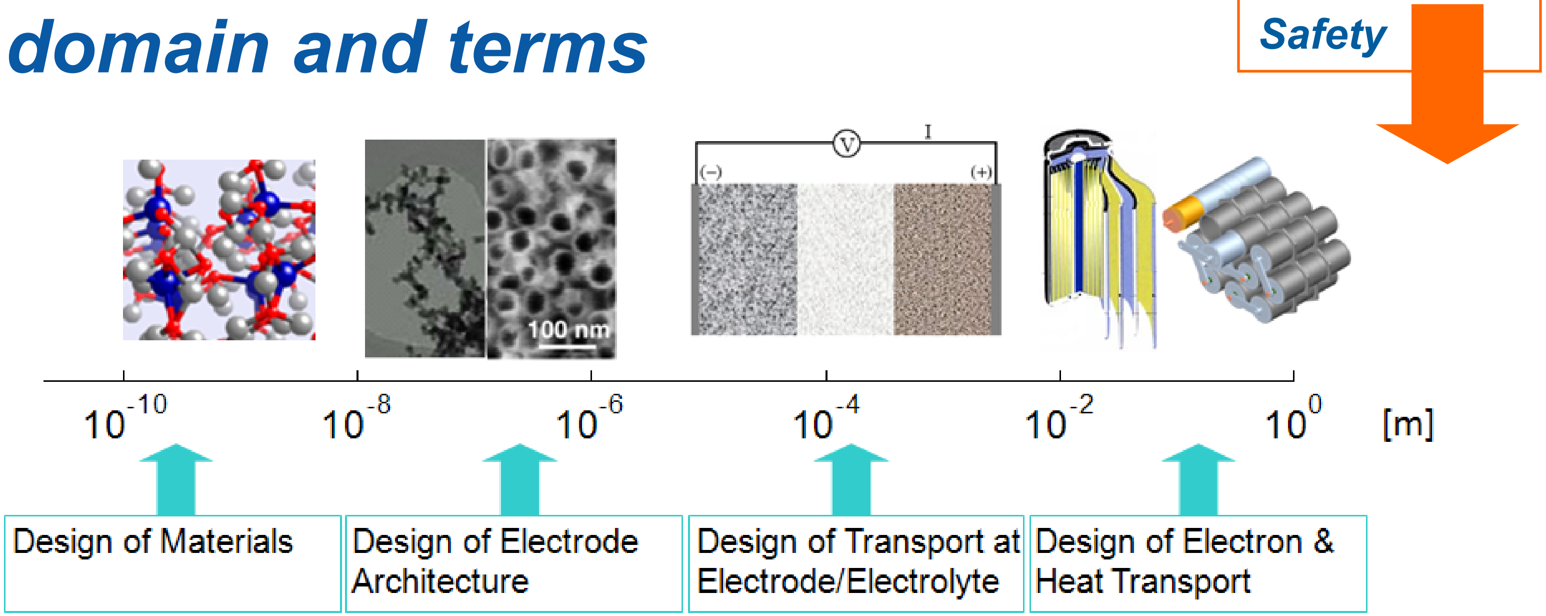
Process Integration, Design & Optimization (PIDO)Software

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



Performance
Life
Cost
Safety

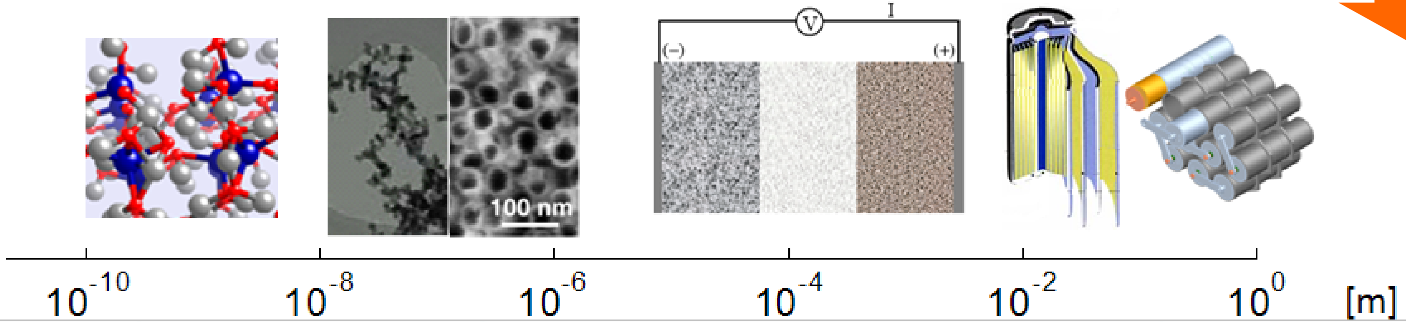
Design of Materials	Design of Electrode Architecture	Design of Transport at Electrode/Electrolyte	Design of Electron & Heat Transport

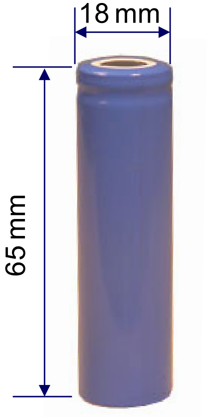
- Wide range of length and time scale physics
- Design improvements required at different scales
- Need for better understanding of interaction among different scale physics

Multi-Scale Physics in Li-Ion Battery

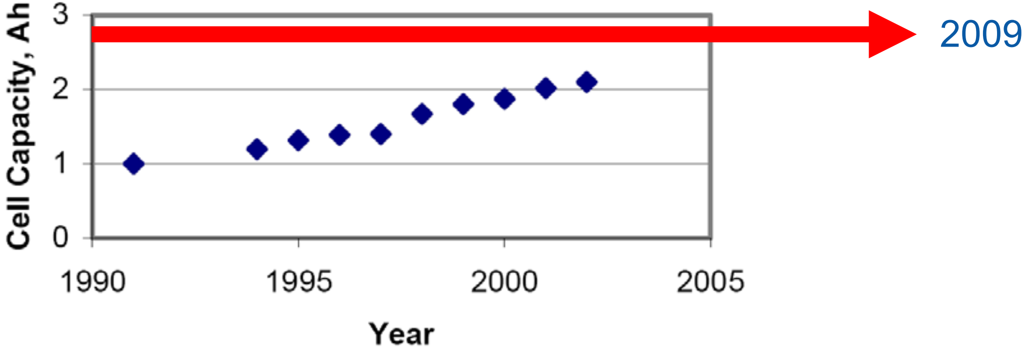
“Requirements” are usually defined in a macroscale domain and terms

Performance
Life
Cost
Safety





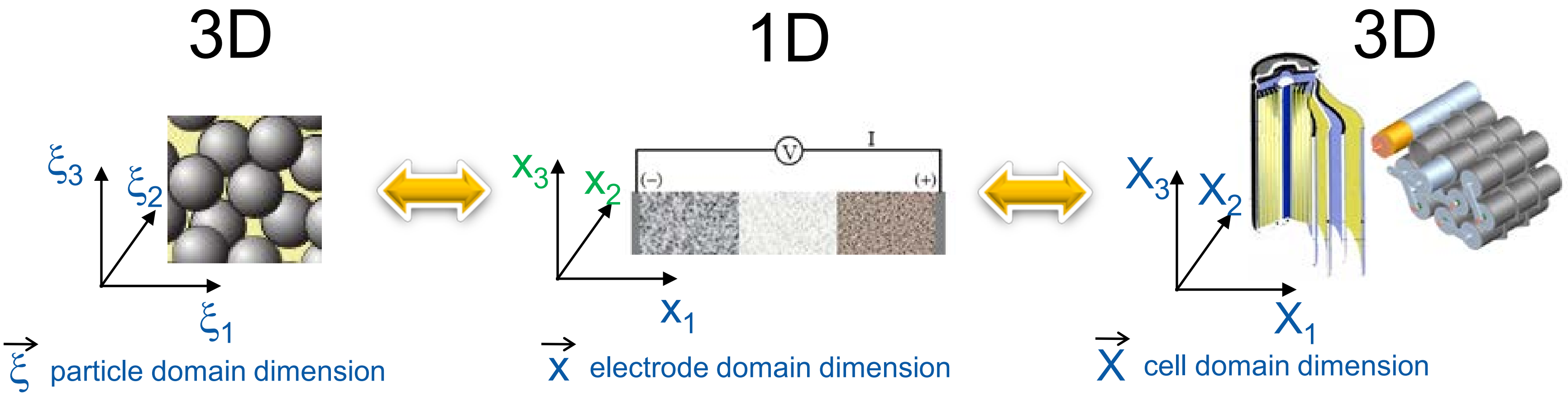
Capacity Increase of commercial 18650 Li-ion cells



www.electrochem.org/dl/ma/201/pdfs/0259.pdf

NREL’s Multi-Scale Multi-Dimensional Model Approach

Efficient representation of 3D electrochemical/thermal physics



3D

1D

3D

$\vec{\xi}$ particle domain dimension

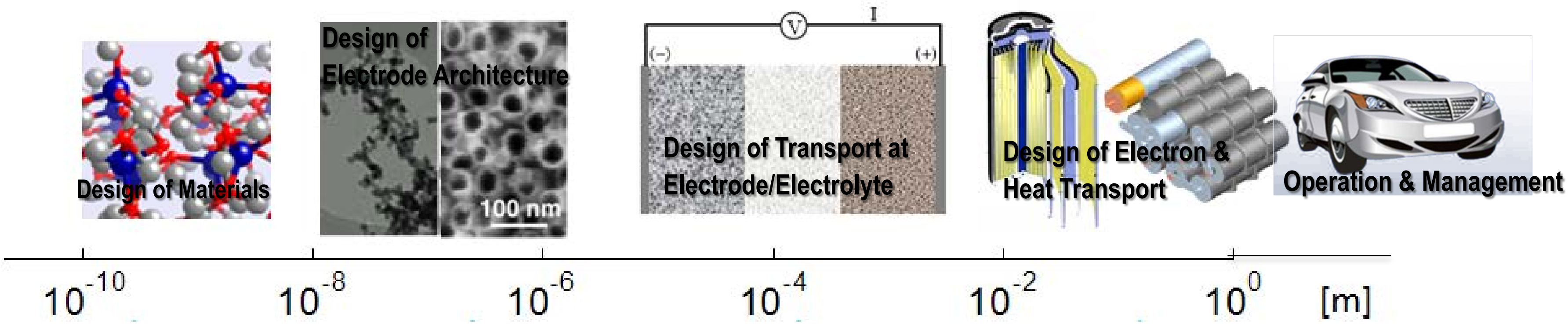
$\vec{x}$ electrode domain dimension

$\vec{X}$ cell domain dimension

NREL

MSMD-μ

MSMD-c



Design of Materials

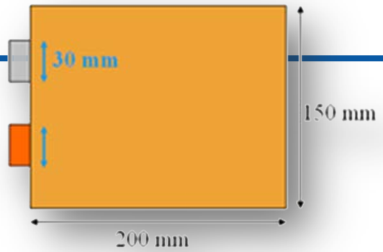
Design of Electrode Architecture

Design of Transport at Electrode/Electrolyte

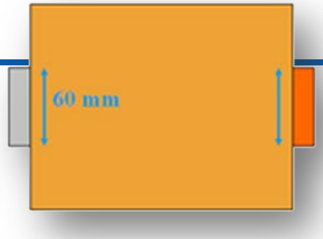
Design of Electron & Heat Transport

Operation & Management

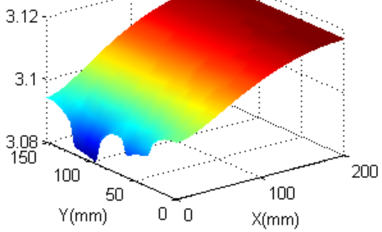
Importance of Multi-Physics Interaction



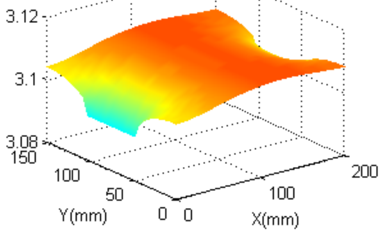
Comparison of two 40 Ah
flat cell designs
2 min 5C discharge



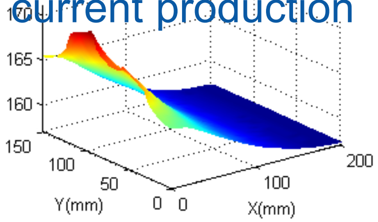
working potential



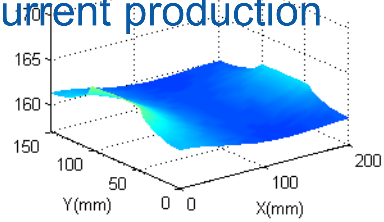
working potential



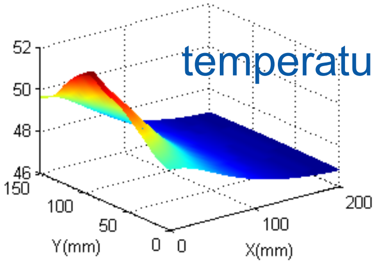
electrochemical current production



electrochemical current production



temperature



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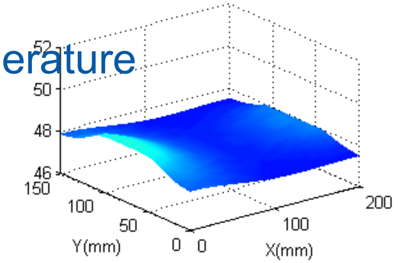
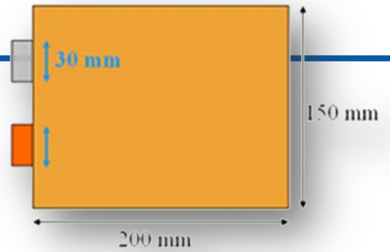
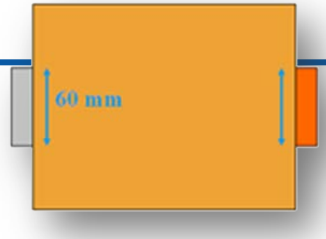


Importance of Multi-Physics Interaction

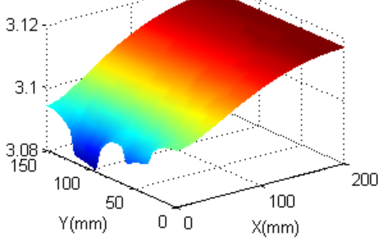


Comparison of two 40 Ah
flat cell designs
2 min 5C discharge

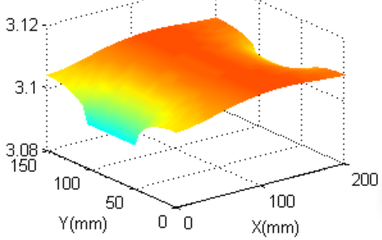


- *Larger over-potential promotes faster discharge reaction*
- *Converging current causes higher potential drop along the collectors*

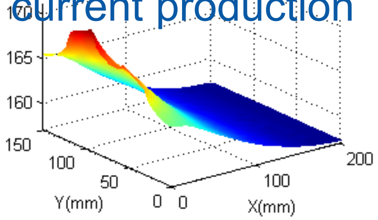
working potential



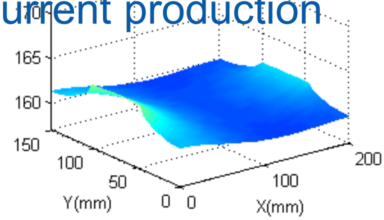
working potential



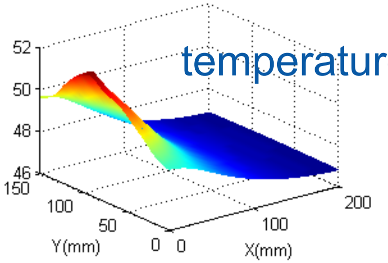
electrochemical current production



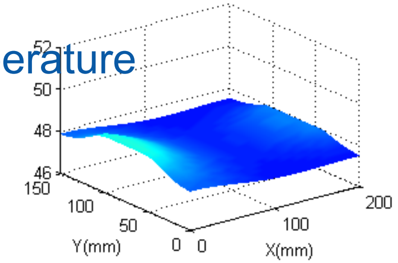
electrochemical current production



temperature



temperature



Importance of Multi-Physics Interaction

Comparison of two 40 Ah
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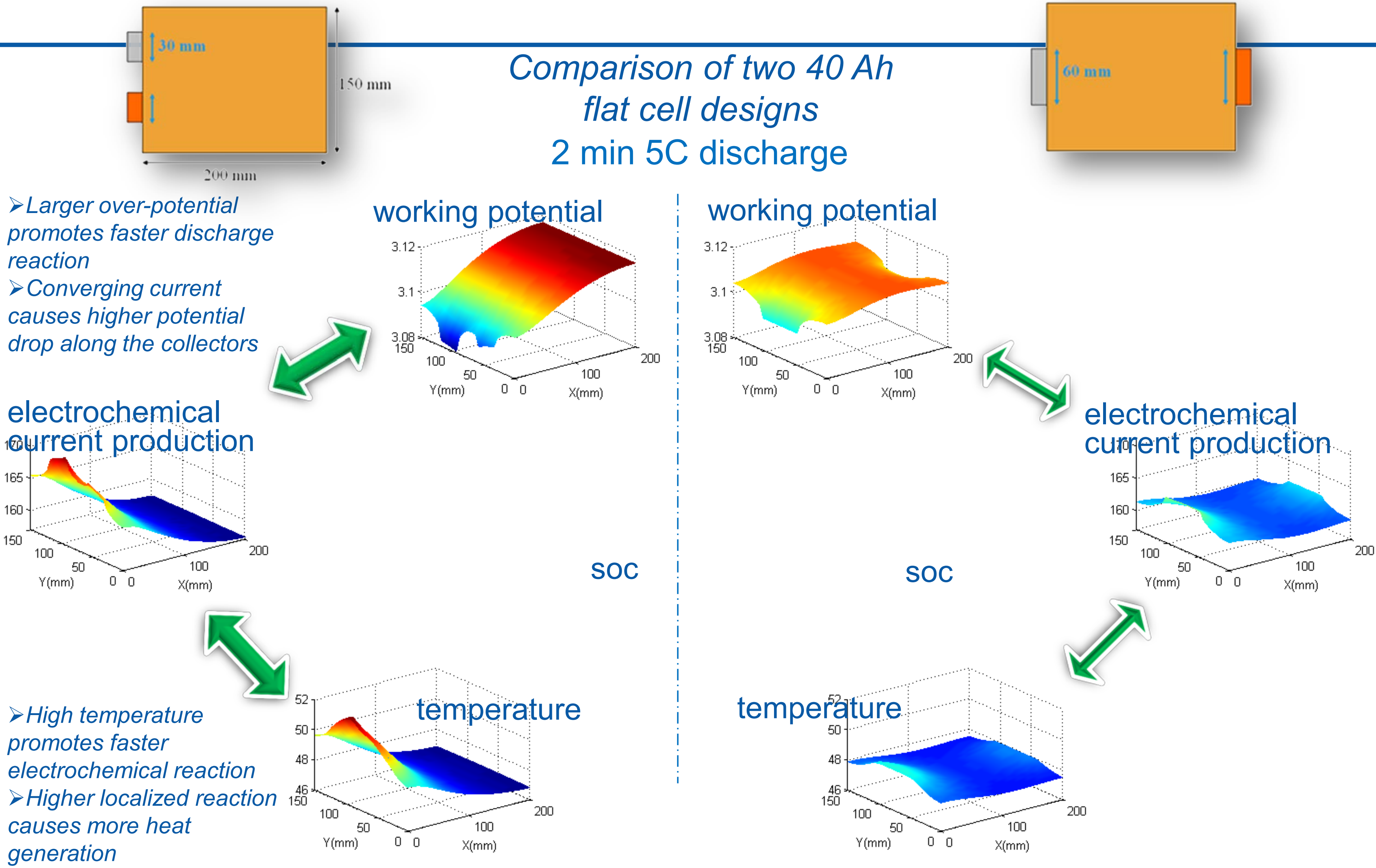
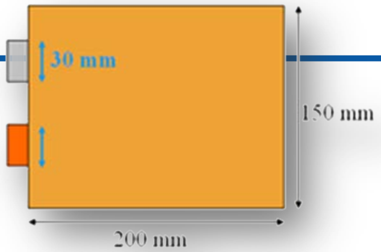


- *Larger over-potential promotes faster discharge reaction*
- *Converging current causes higher potential drop along the collectors*

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

Importance of Multi-Physics Interaction



Comparison of two 40 Ah
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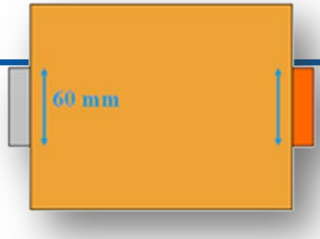

- *Larger over-potential promotes faster discharge reaction*
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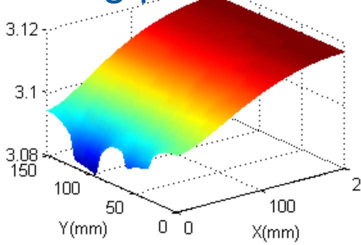
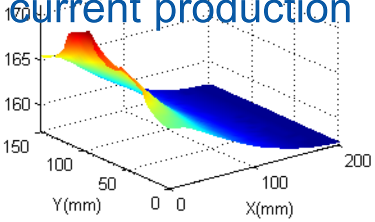
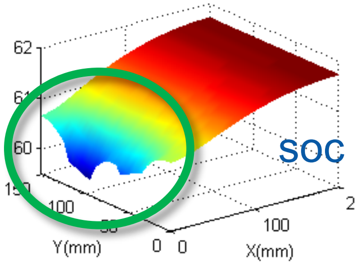


electrochemical current production

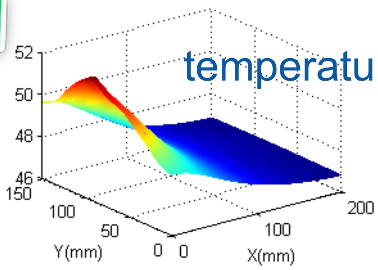




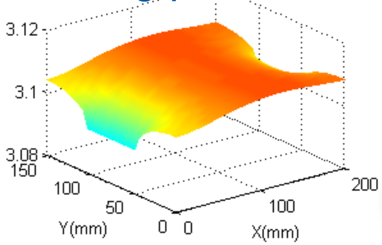
SOC

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

temperature

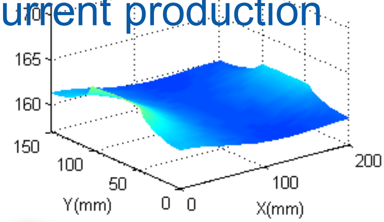


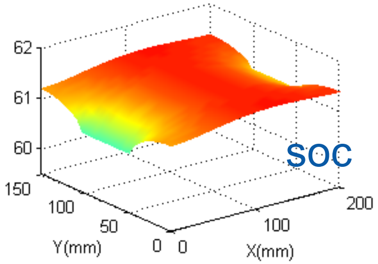
working potential



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

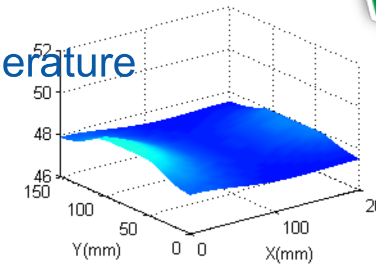
electrochemical current production





SOC

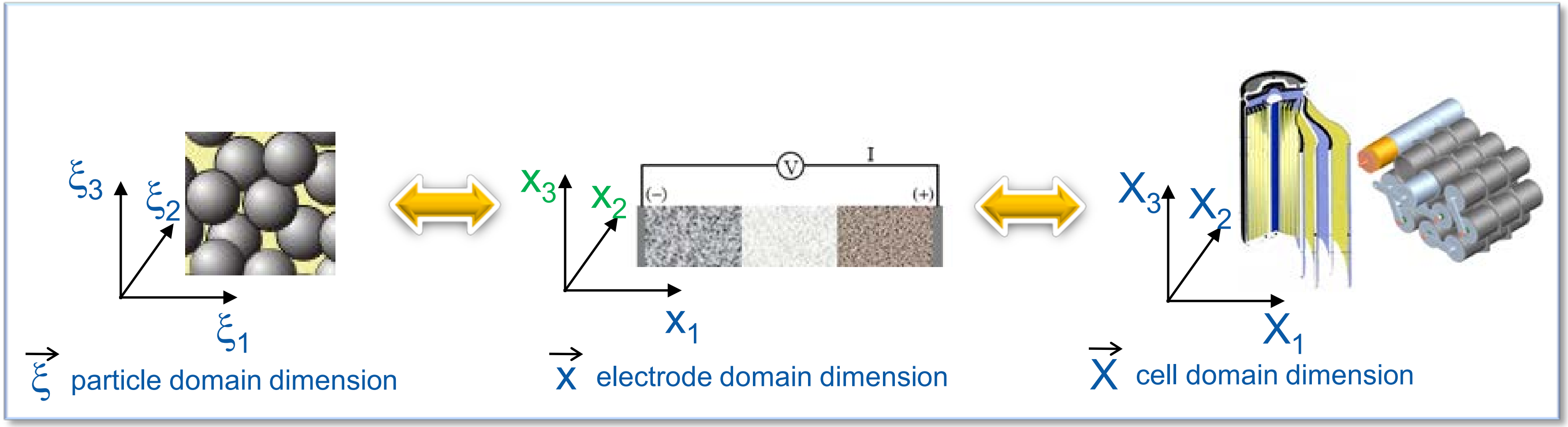
temperature



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

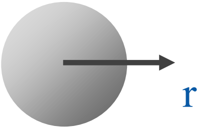


$\vec{\xi}$ particle domain dimension

$\vec{x}$ electrode domain dimension

$\vec{X}$ cell domain dimension

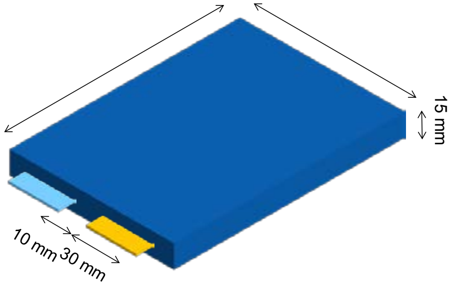
1D



1D

SVM

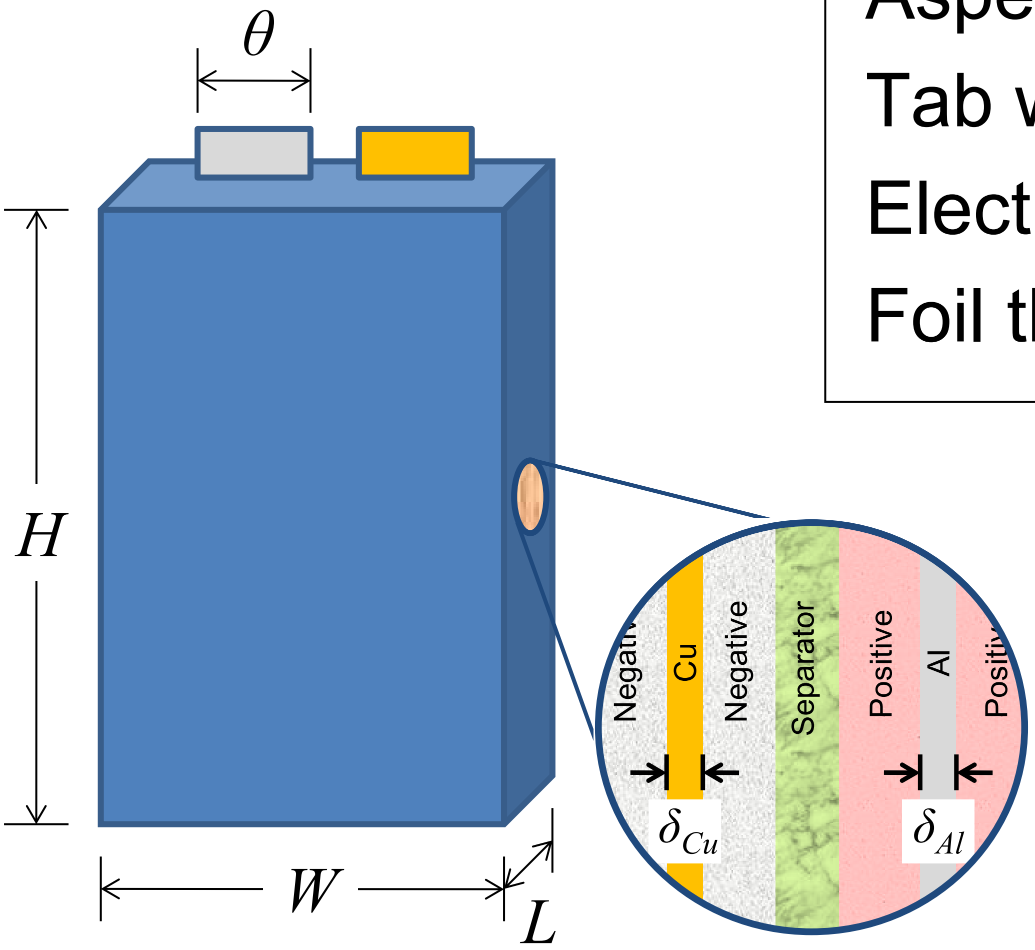
2D



- ✓ *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:

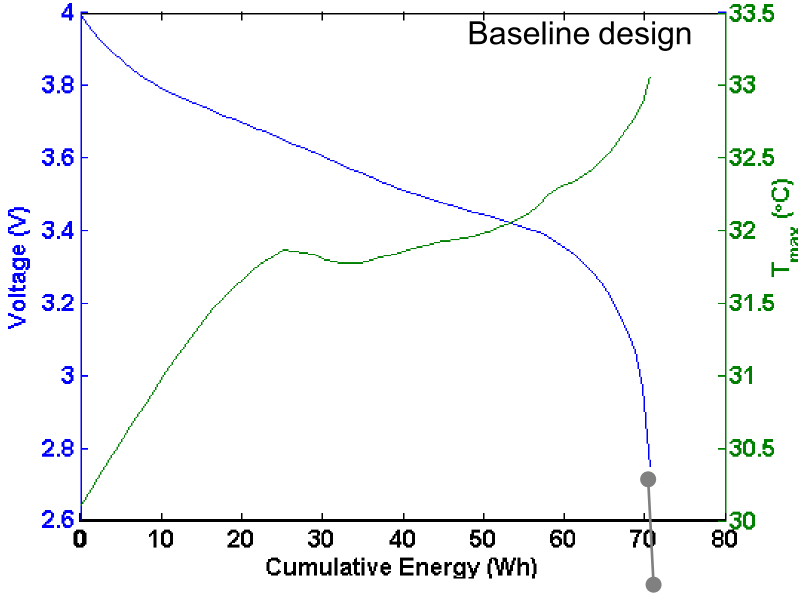
- $\delta_{Al} = 1.6 \times \delta_{Cu}$
- 20 Ah capacity
- Electrode loadings
- Electrode thicknesses

(Typical tradeoff between power & energy do not arise in this study)

Cell Design Evaluation Criteria

Energy at 2C rate

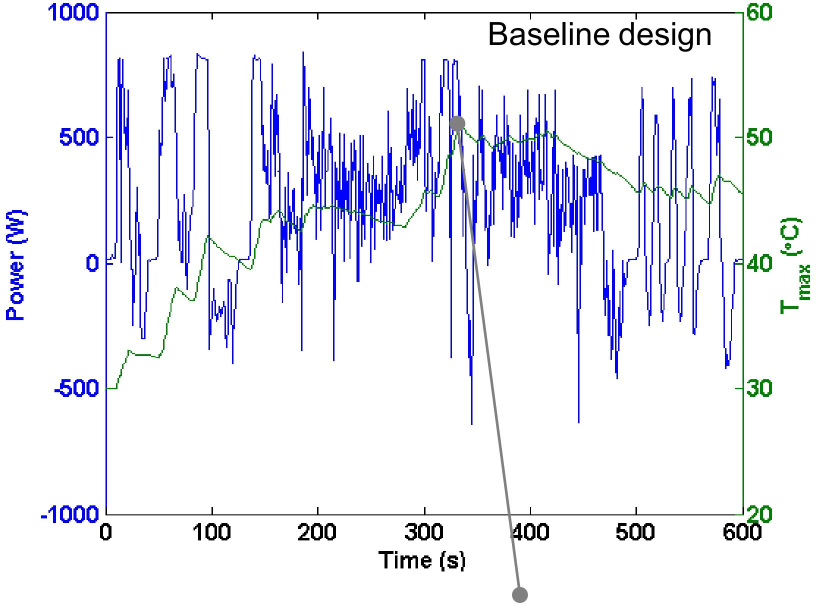
- Energy density (Wh/L) evaluated at module level (includes 5mm external tab height + 3 mm cooling channel between cells)



71 Wh

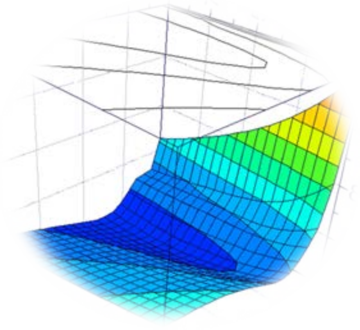
Maximum temperature during driving cycle

- 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) Tmax (Nlayers, t_CU, H_W, tTab_W)
   b) Energy_Density (Nlayers, t_CU, H_W, tTab_W)
   c) Specific_Energy (Nlayers, t_CU, H_W, tTab_W)
   d) Cell Thickness (Nlayers, t_CU, H_W, tTab_W)

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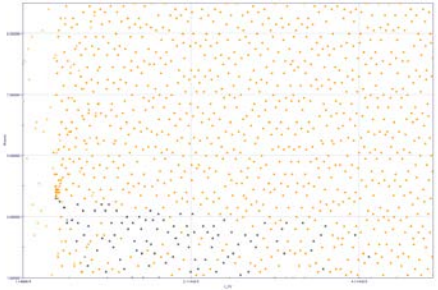

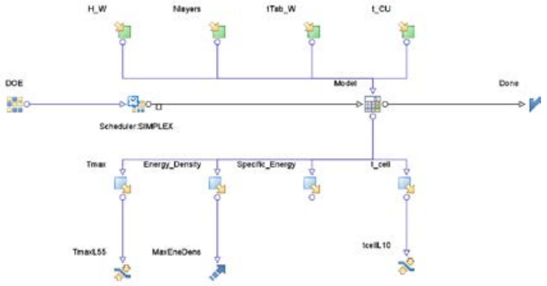

Optimization Process Steps - 2

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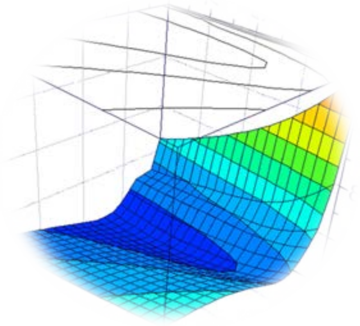
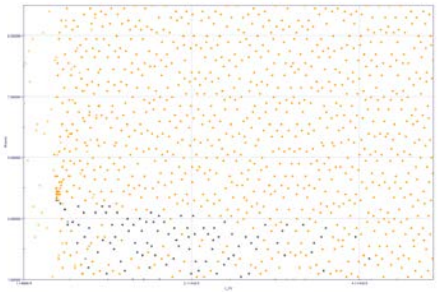
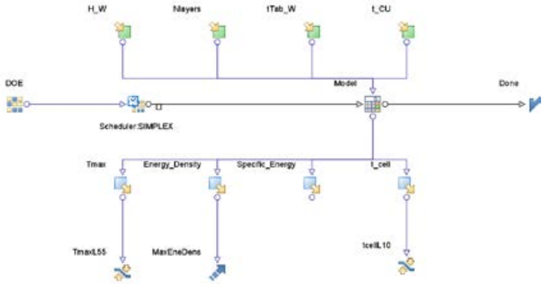
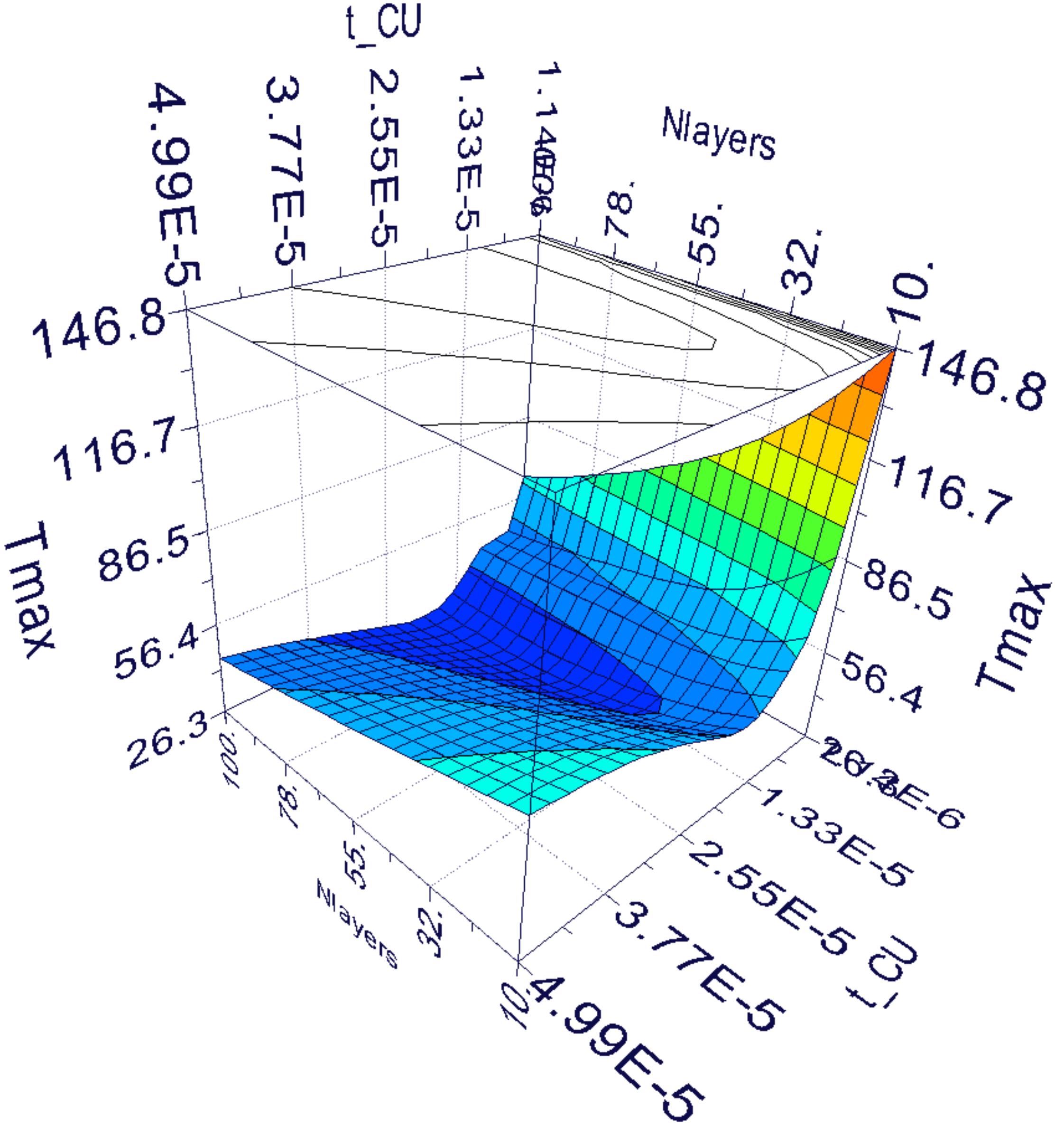


4. Generate 1000 more DOE points using a simple sampling technique (Sobol)
5. Run the 1000 DOE points through the 4 response functions to generate 1000 more data points
6. Select the best of the 1050 design points and use it as starting point for an optimization algorithm
7. The optimizer tries to maximize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

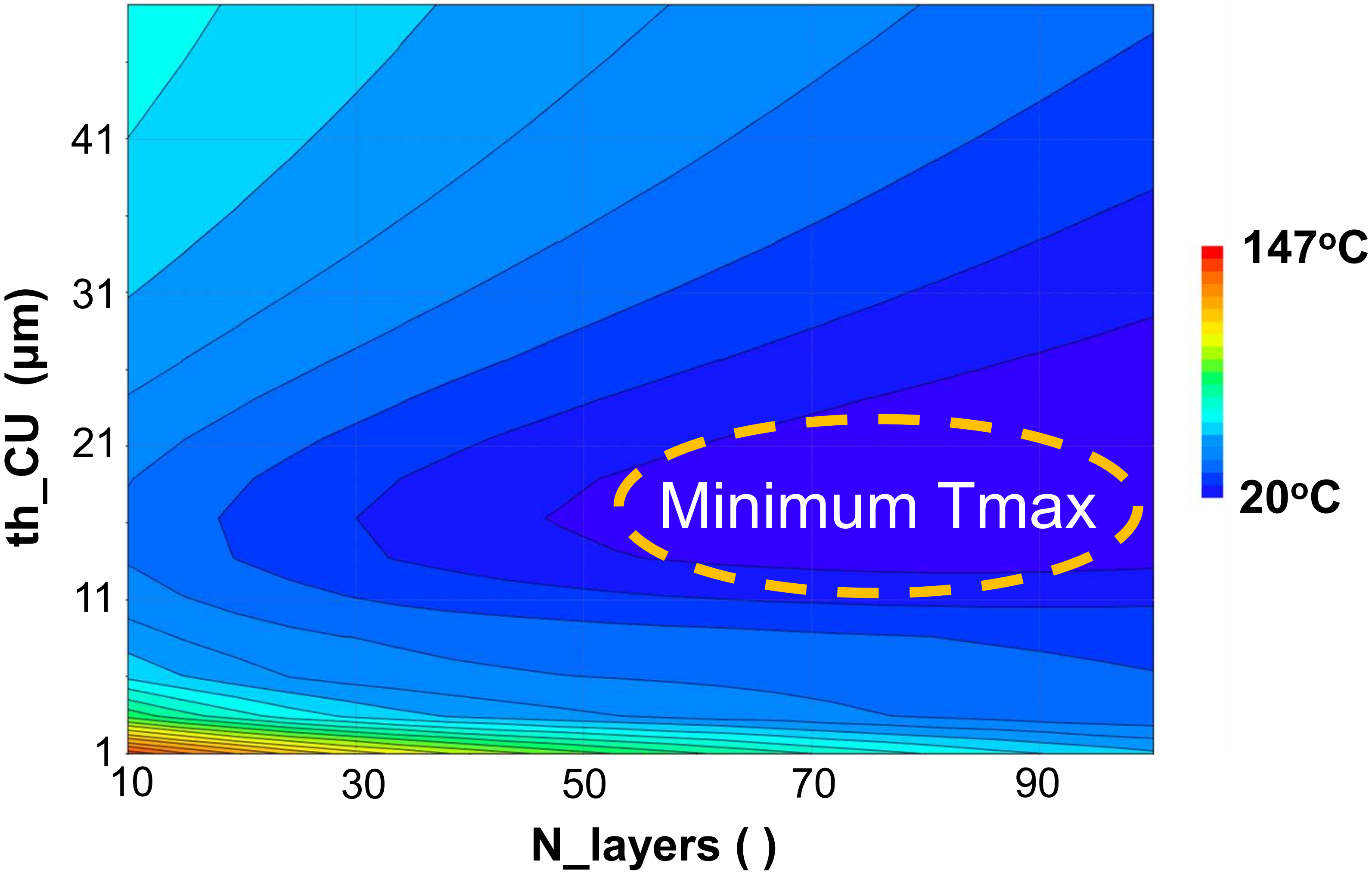




Tmax Response Surface versus Number of Layers & Cu Foil Thickness



Tmax versus Number of Layers & Cu Foil Thickness



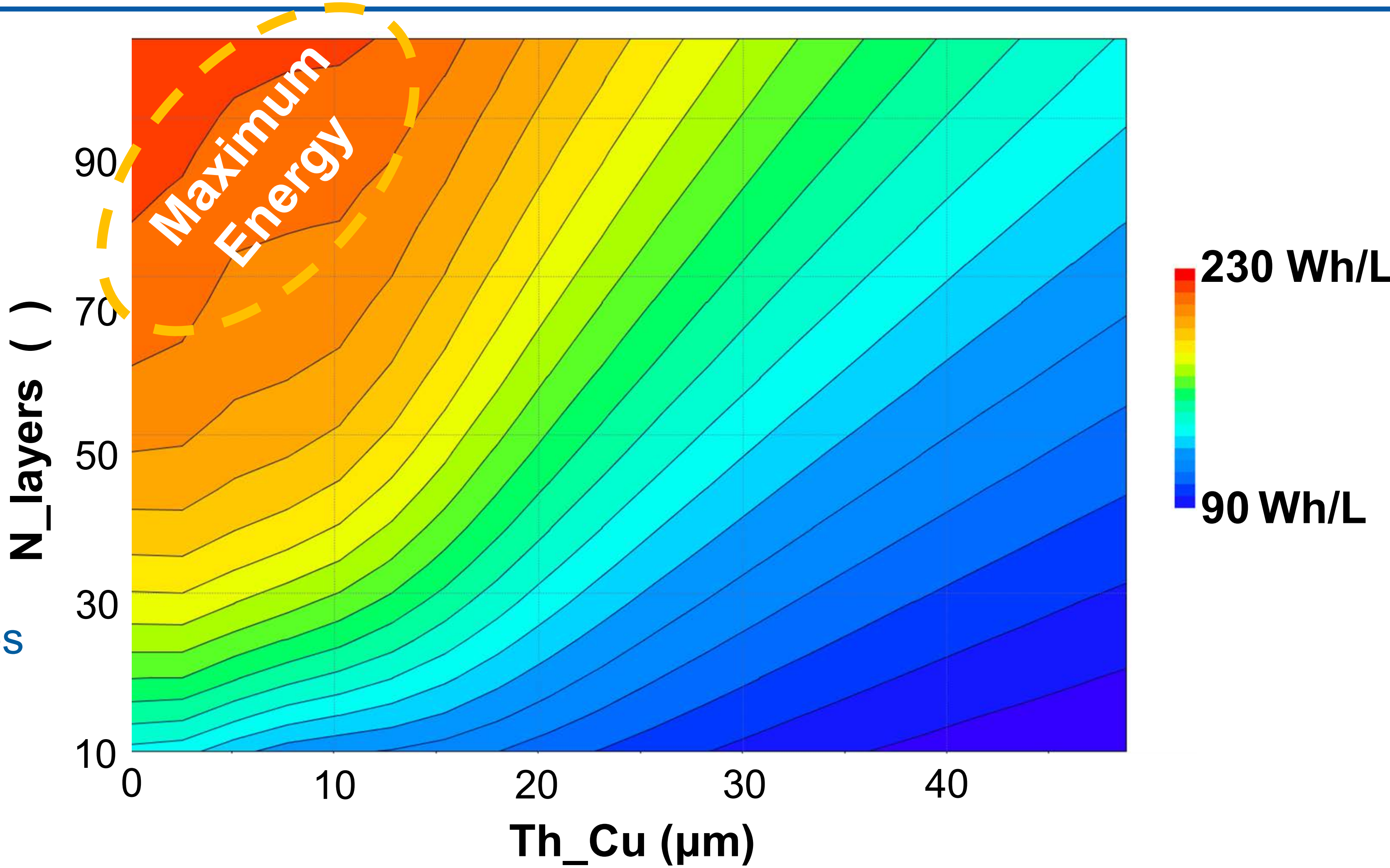
Thinner foil shortens thermal diffusion length

Thicker foil reduces ohmic losses

More layers reduces Tmax by creating shorter, parallel paths for e$^-$ flow

Energy Density* versus Number of Layers & Cu Foil Thickness

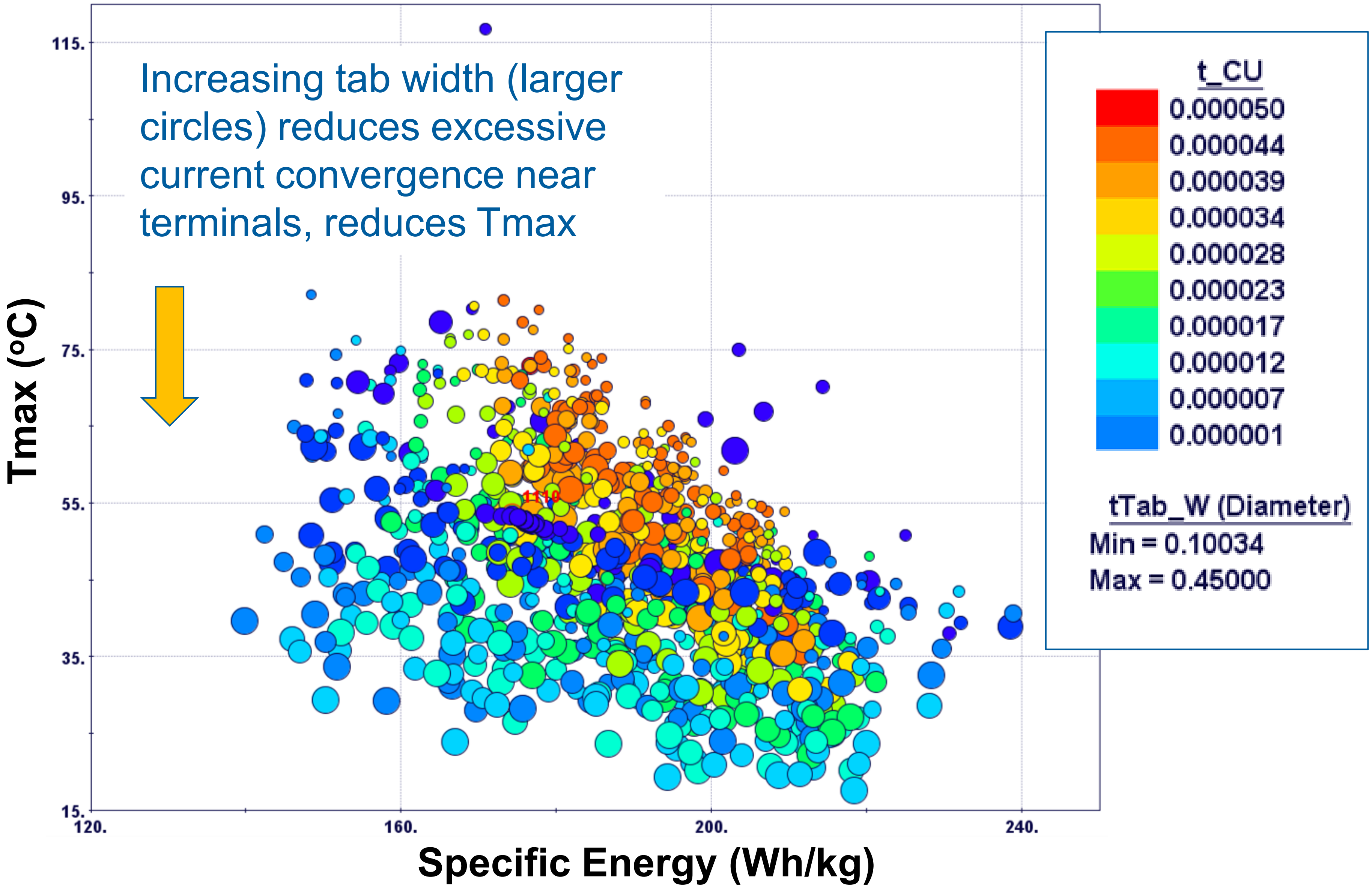
More parallel layers reduces losses, maximizes useable energy



Less foil reduces volume, mass of inert components

*2C rate, module level Wh/L

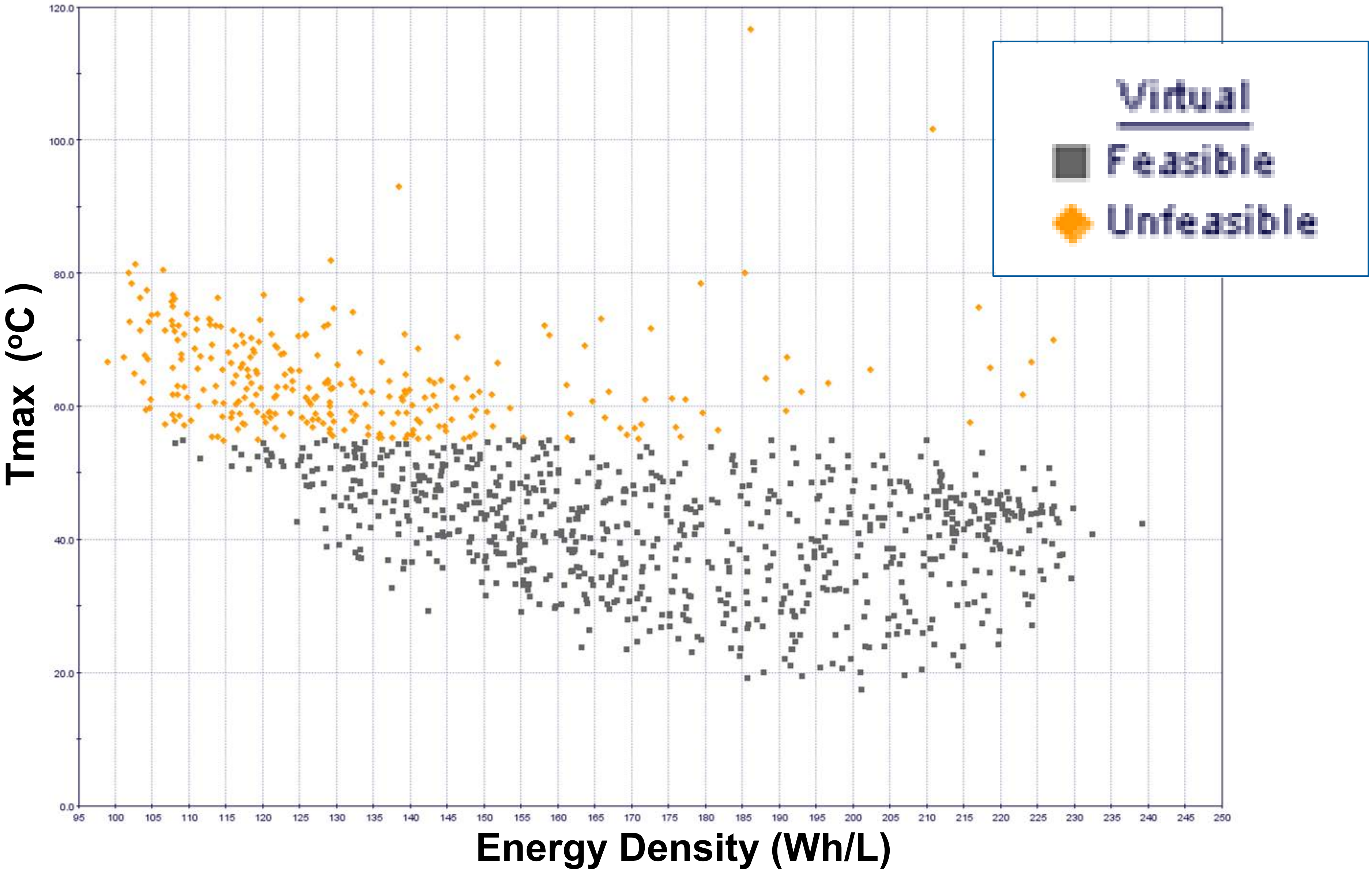
Scatter Plot of Tmax versus Specific Energy
for various values of Cu thickness and tab width ratio



Increasing tab width (larger circles) reduces excessive current convergence near terminals, reduces Tmax

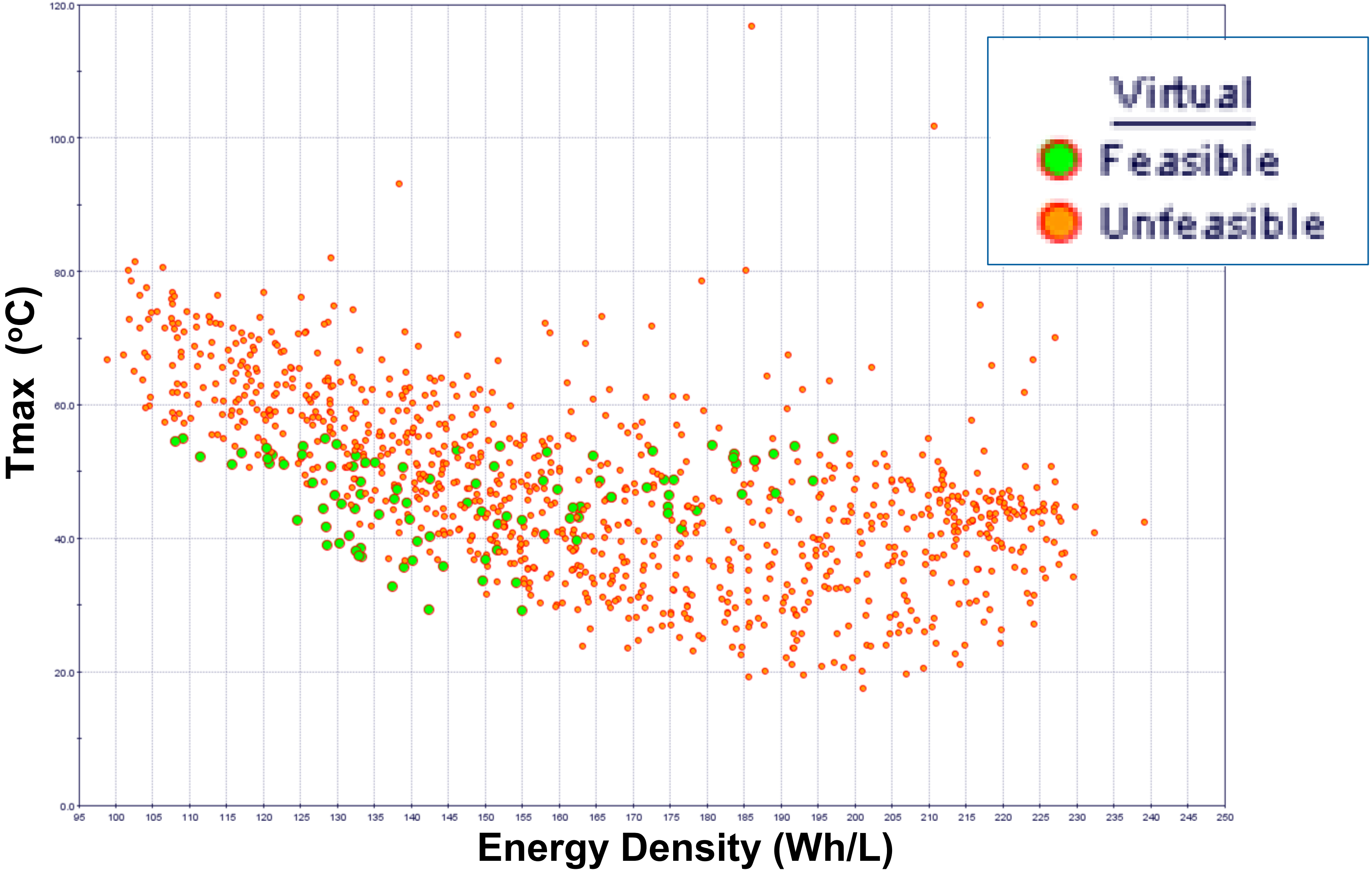
Scatter Plot of Tmax versus Energy Density

Feasible points with Tmax < 55^{o}C

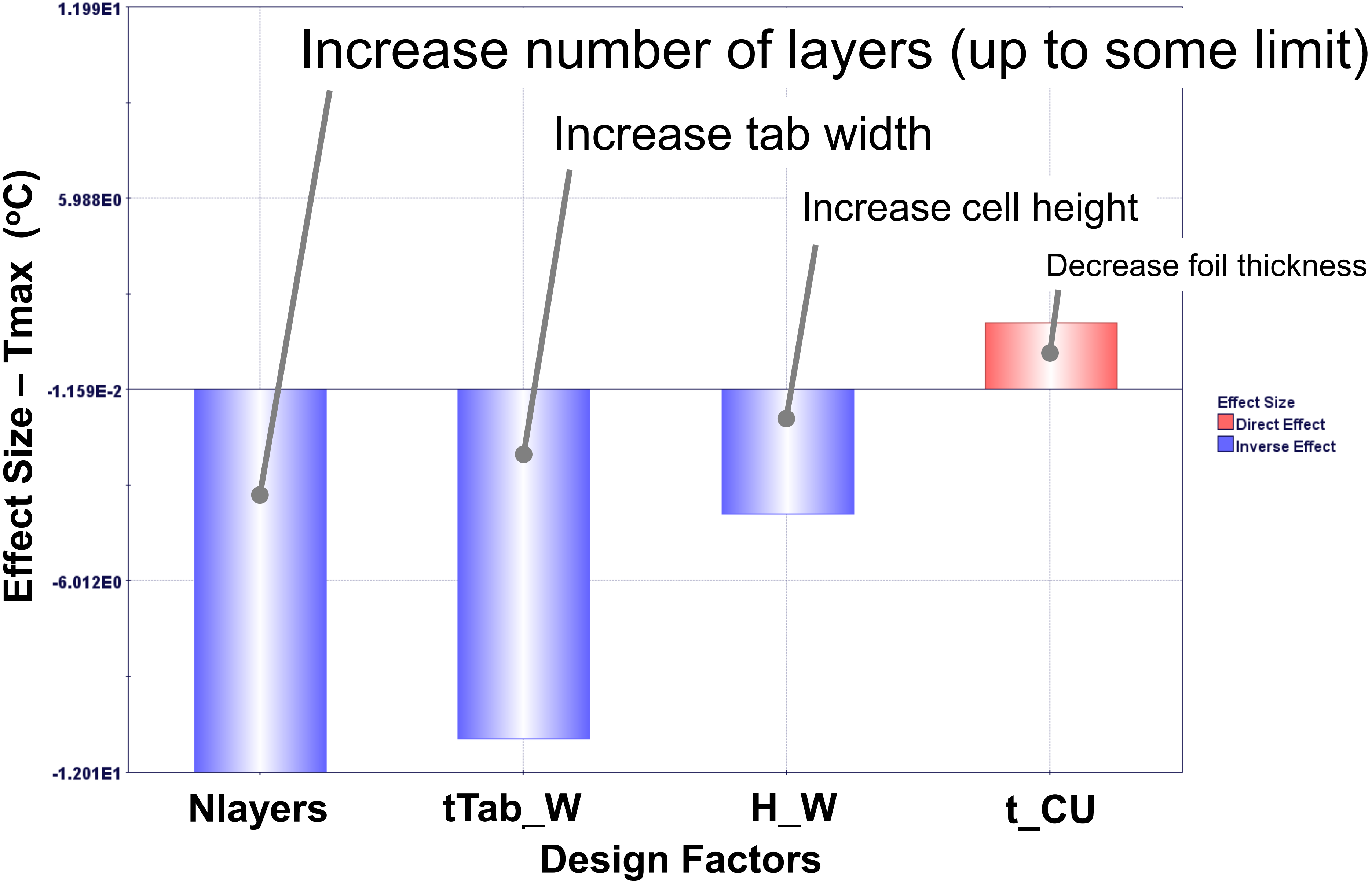


Scatter Plot of Tmax versus Energy Density

Feasible points with Tmax < 55^{o}C and Cell thickness < 16 mm



Effect of Design Variables on Tmax (minimize)

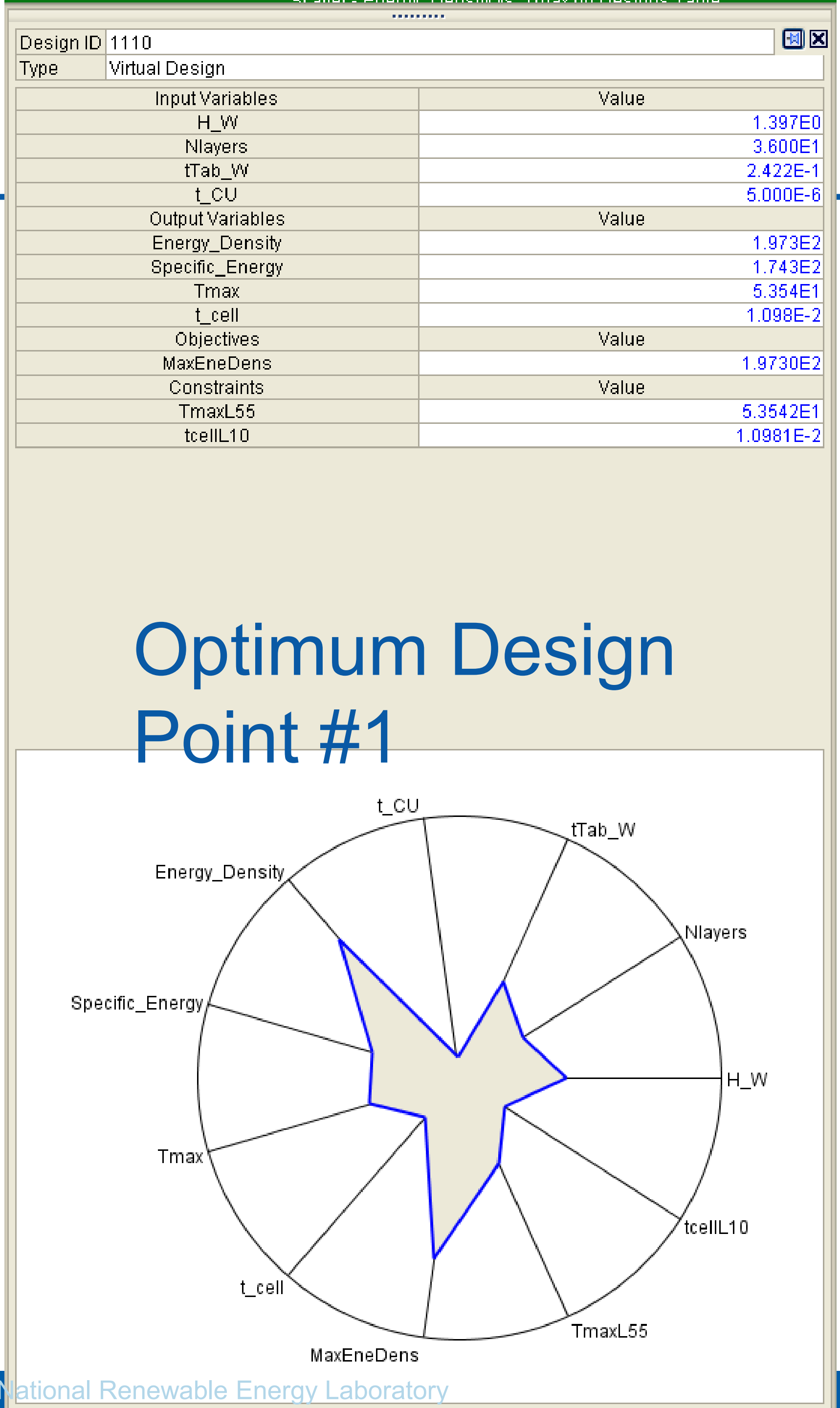


Increase number of layers (up to some limit)

Increase tab width

Increase cell height

Decrease foil thickness



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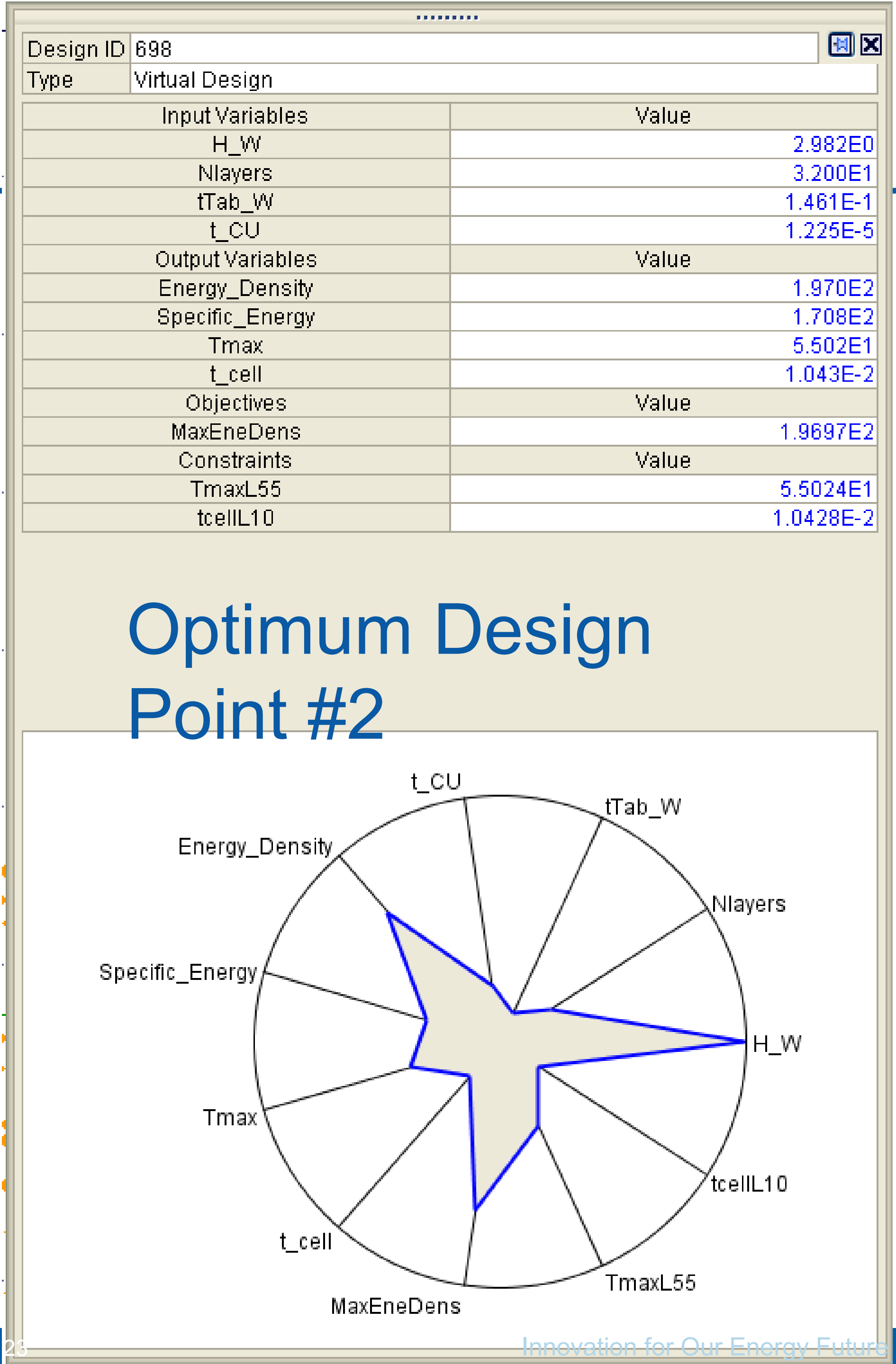
Type	Virtual Design

Input Variables	Value
H_W	1.397E0
Nlayers	3.600E1
tTab_W	2.422E-1
t_CU	5.000E-6
Output Variables	**Value**
Energy_Density	1.973E2
Specific_Energy	1.743E2
Tmax	5.354E1
t_cell	1.098E-2
Objectives	**Value**
MaxEneDens	1.9730E2
Constraints	**Value**
TmaxL55	5.3542E1
tcellL10	1.0981E-2

Optimum Design Point #1



Design ID	698
Type	Virtual Design

Input Variables	Value
H_W	2.982E0
Nlayers	3.200E1
tTab_W	1.461E-1
t_CU	1.225E-5
Output Variables	**Value**
Energy_Density	1.970E2
Specific_Energy	1.708E2
Tmax	5.502E1
t_cell	1.043E-2
Objectives	**Value**
MaxEneDens	1.9697E2
Constraints	**Value**
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 (°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

→

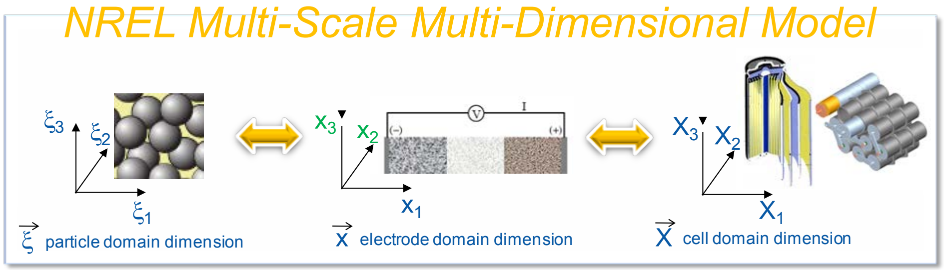
Improved energy density

Peak temperatures reduced 10°C

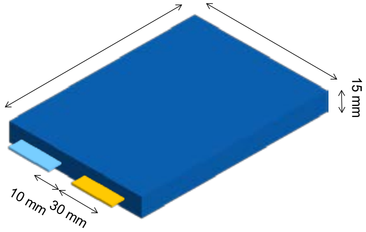
*module level energy density includes 5mm external tab height & fixed 3mm intercell gap

Conclusions

- Large cell design is challenging problem of competing requirements & objectives
- Robust design CAE methods provide straight-forward process for optimization, so long as
  - Objectives & constraints are well-defined
  - Physics and geometry are properly captured


NREL Multi-Scale Multi-Dimensional Model

- Compared to baseline design, optimization of macroscopic factors decreases peak temperatures (fewer losses in cell) while increasing useable energy density



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