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Innovation for Our Energy Future

Evaluation Study for Large Prismatic Lithium-Ion Cell Designs Using Multi-Scale Multi-Dimensional Battery Model

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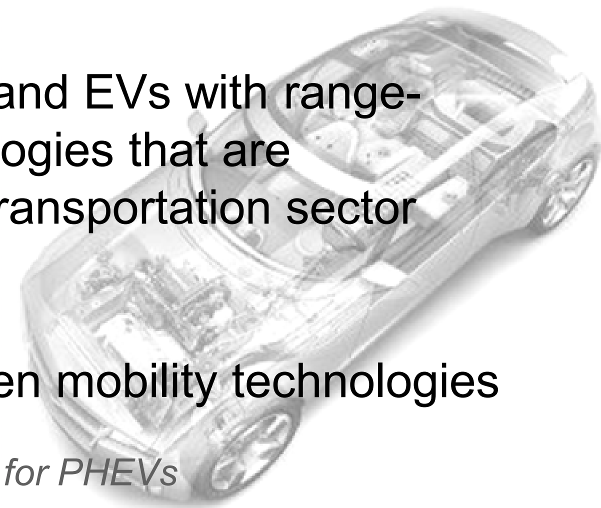
Batteries for Electrified Vehicles



Electrified drive-train vehicles such as PHEVs and EVs with range-extenders are believed to be near-term technologies that are

- displacing significant petroleum use in the transportation sector
- diversifying energy sources for mobility

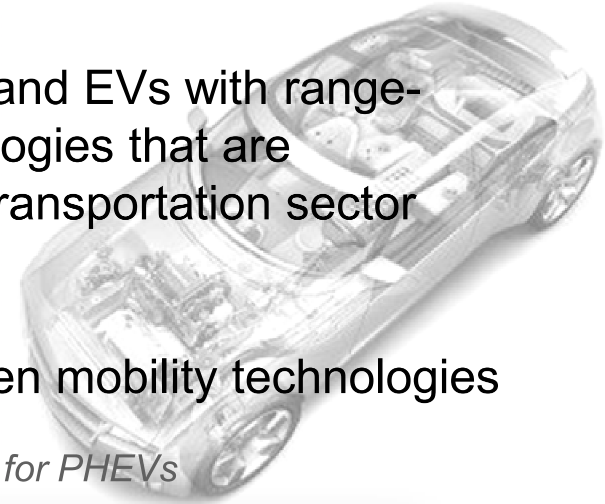
Advances in batteries are critical to realize green mobility technologies

DOE's Energy Storage System Performance Targets for PHEVs

Table 1. Energy Storage System Performance Targets for Plug-In Hybrid Electric Vehicles (January 2007).

Characteristics at EOL (End-of-Life)	Unit	Minimum PHEV Battery	Maximum PHEV Battery
Reference Equivalent Electric Range	miles	10	40
Peak Discharge Pulse Power (2 sec / 10 sec) [1]	kW	50/45	46/38
Peak Regen Pulse Power (10 sec)	kW	30	25
Max. Current (10 sec pulse)	A	300	300
Available Energy for CD (Charge-Depleting) Mode, 10-kW Rate	kWh	3.4	11.6
Available Energy for CS (Charge-Sustaining) Mode, 10-kW Rate [2]	kWh	0.5	0.3
Minimum Round-trip Energy Efficiency (CS 50 Wh profile)	%	90	90
Cold cranking power at -30°C, 2 sec, 3 Pulses	kW	7	7
CD Life / Discharge Throughput	Cycles/MWh	5,000 / 17	5,000 / 58
CS HEV Cycle Life, 50 Wh Profile	Cycles	300,000	300,000
Calendar Life, 35°C	year	15	15
Maximum System Weight	kg	60	120
Maximum System Volume	Liter	40	80
Maximum Operating Voltage	Vdc	400	400
Minimum Operating Voltage	Vdc	>0.55 x Vmax [3]	>0.55 x Vmax [3]
Maximum Self-discharge	Wh/day	50	50
Maximum System Recharge Rate at 30°C	kW	1.4 (120V/15A) [4]	1.4 (120V/15A) [4]
Unassisted Operating & Charging Temperature Range 52°C >100% Available Power 0°C >50% Available Power -10°C >30% Available Power -30°C >10% Available Power	°C	-30 to +52	-30 to +52
Survival Temperature Range	°C	-46 to +66	-46 to +66
Maximum System Production Price @ 100k units/yr	$	$1,700	$3,400

Batteries for Electrified Vehicles



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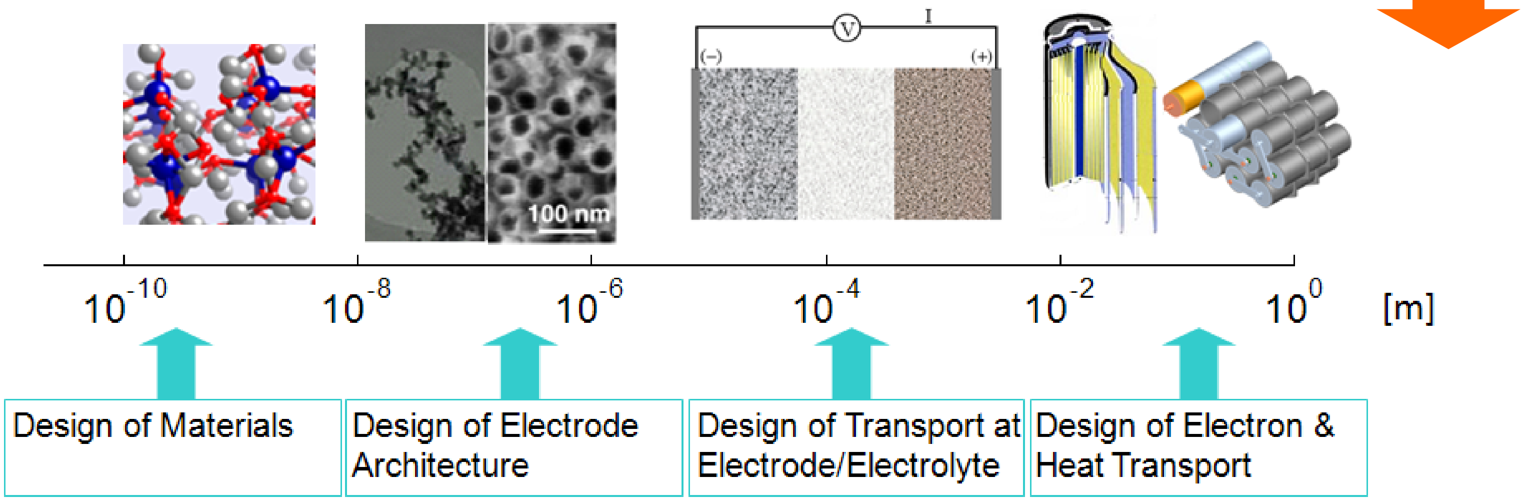
Performance
Life
Cost
Safety

Multi-Scale Physics in Li-Ion Battery

Requirements & Resolutions

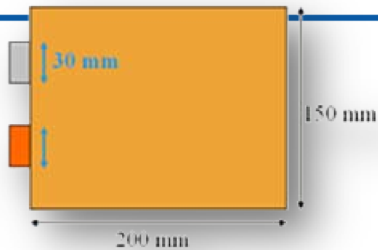
"Requirements" are usually defined in a macroscale domain and terms

Performance
Life
Cost
Safety



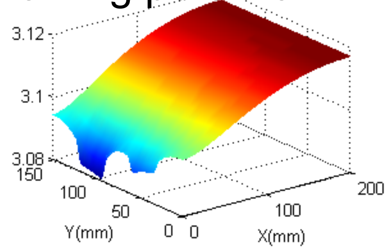
- Wide range of length and time scale physics
- Design improvements required at different scales
- Need for better understanding of interaction among different scale physics

Multi-Physics Interaction



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

working potential



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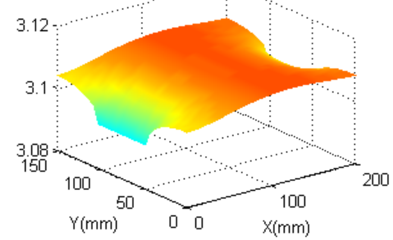
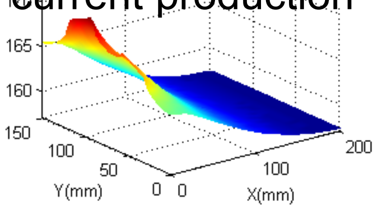


electrochemical current production



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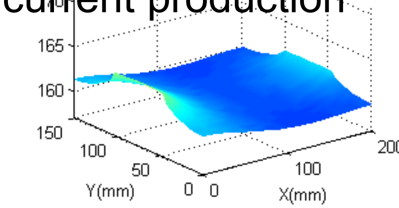
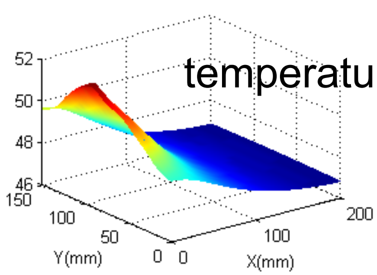


temperature



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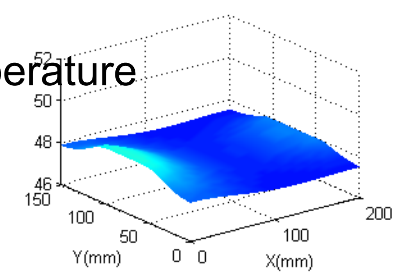

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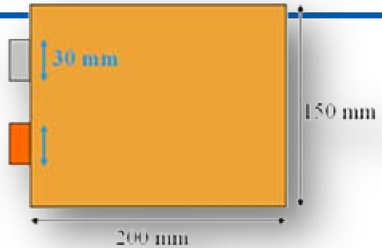

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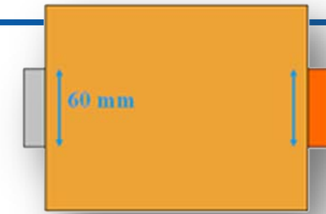
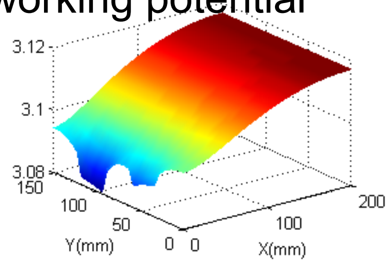


- *Larger over-potential promotes faster discharge reaction*
- *Converging current causes higher potential drop along the collectors*

working potential



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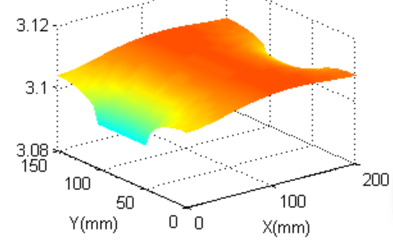
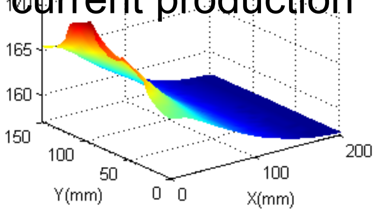


electrochemical current production



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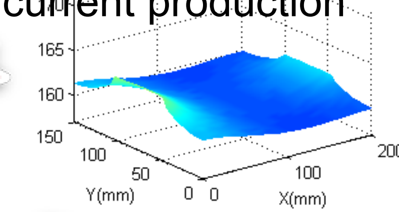
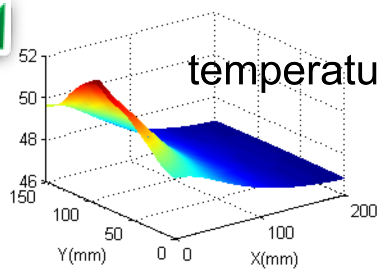
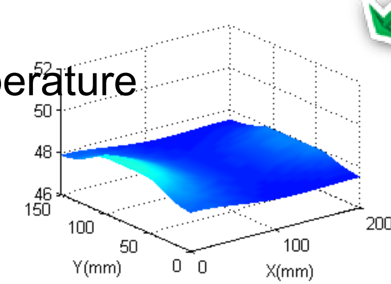


- *High temperature promotes faster electrochemical reaction*
- *Higher localized reaction causes more heat generation*

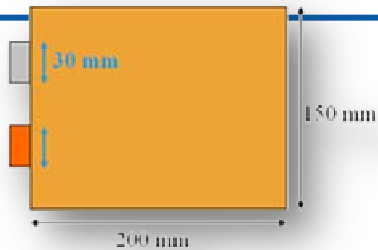
temperature



temperature



Multi-Physics Interaction



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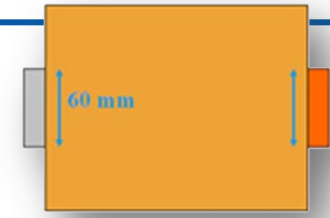
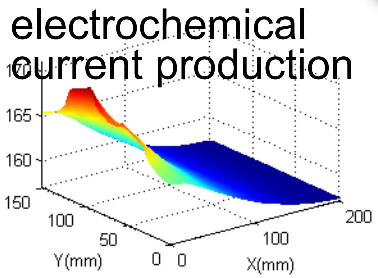
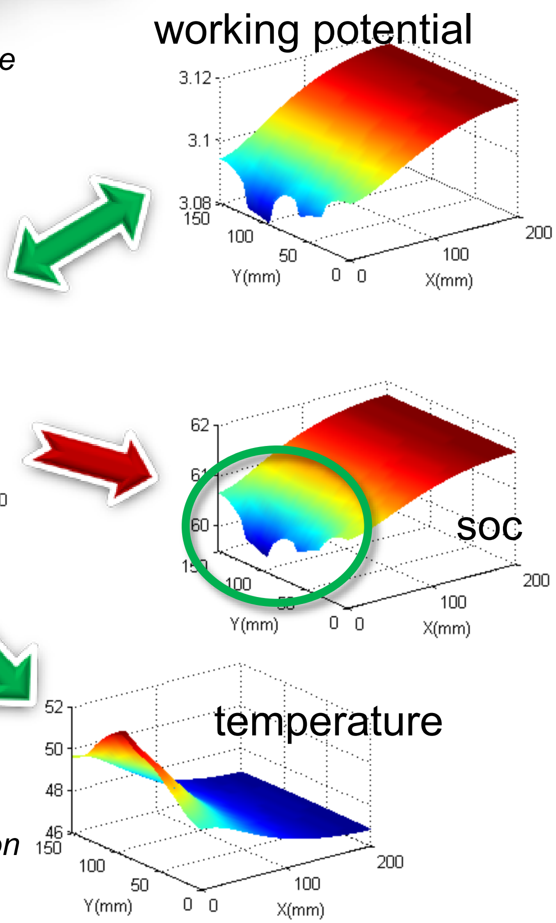


- ➢*Larger over-potential promotes faster discharge reaction*
- ➢*Converging current causes higher potential drop along the collectors*





- ➢*High temperature promotes faster electrochemical reaction*
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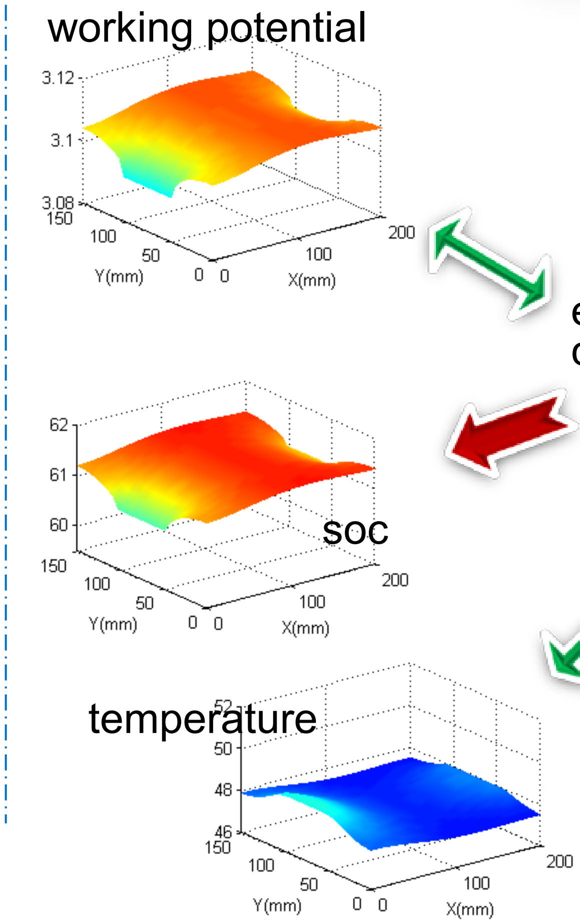
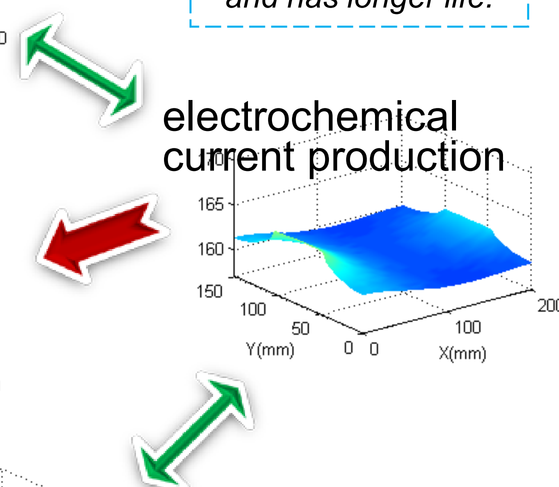
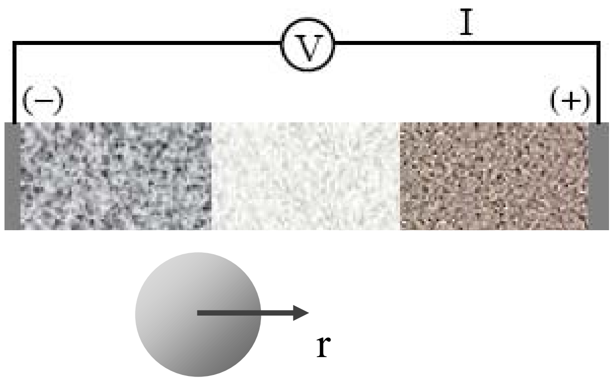


This cell is cycled more uniformly, can therefore use less active material ($) and has longer life.



Electrode-Scale Performance Model



Charge Transfer Kinetics at Reaction Sites

$$j^{Li} = a_s i_o \left\{ \exp\left[\frac{\alpha_a F}{RT}\eta\right] - \exp\left[-\frac{\alpha_c F}{RT}\eta\right] \right\}$$

$$i_0 = k(c_e)^{\alpha_a}(c_{s,\max} - c_{s,e})^{\alpha_a}(c_{s,e})^{\alpha_c} \qquad \eta = (\phi_s - \phi_e) - U$$

Species Conservation

$$\frac{\partial c_s}{\partial t} = \frac{D_s}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial c_s}{\partial r}\right)$$

$$\frac{\partial(\varepsilon_e c_e)}{\partial t} = \nabla \cdot \left(D_e^{eff} \nabla c_e\right) + \frac{1 - t_+^o}{F} j^{\mathrm{Li}} - \frac{\mathbf{i}_e \cdot \nabla t_+^o}{F}$$

Charge Conservation

$$\nabla \cdot \left(\sigma^{eff} \nabla \phi_s\right) - j^{\mathrm{Li}} = 0$$

$$\nabla \cdot \left(\kappa^{eff} \nabla \phi_e\right) + \nabla \cdot \left(\kappa_D^{eff} \nabla \ln c_e\right) + j^{\mathrm{Li}} = 0$$

Energy Conservation

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + q'''$$

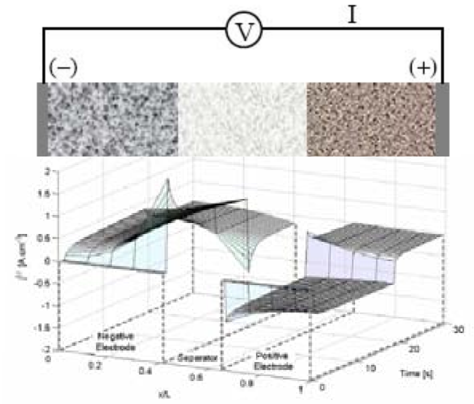
$$q''' = j^{Li}\left(\phi_s - \phi_e - U + T\frac{\partial U}{\partial T}\right) + \sigma^{eff} \nabla \phi_s \cdot \nabla \phi_s + \kappa^{eff} \nabla \phi_e \cdot \nabla \phi_e + \kappa_D^{eff} \nabla \ln c_e \cdot \nabla \phi_e$$

- Pioneered by Newman group (*Doyle, Fuller, and Newman 1993*)
- Captures *lithium diffusion dynamics* and *charge transfer kinetics*
- Predicts *current/voltage response* of a battery
- Provides design guide for thermodynamics, kinetics, and transport across electrodes

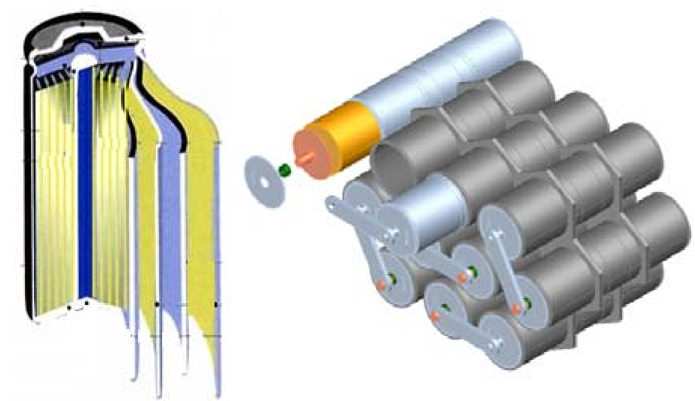
- Difficult to resolve *heat* and *electron current* transport

Integrated Model Resolving Different Scale Physics

To expand knowledge of the impacts of *designs in different scales*, usages, and management on performance, life, and safety of battery systems



Li Transport &
Charge Transfer Kinetics

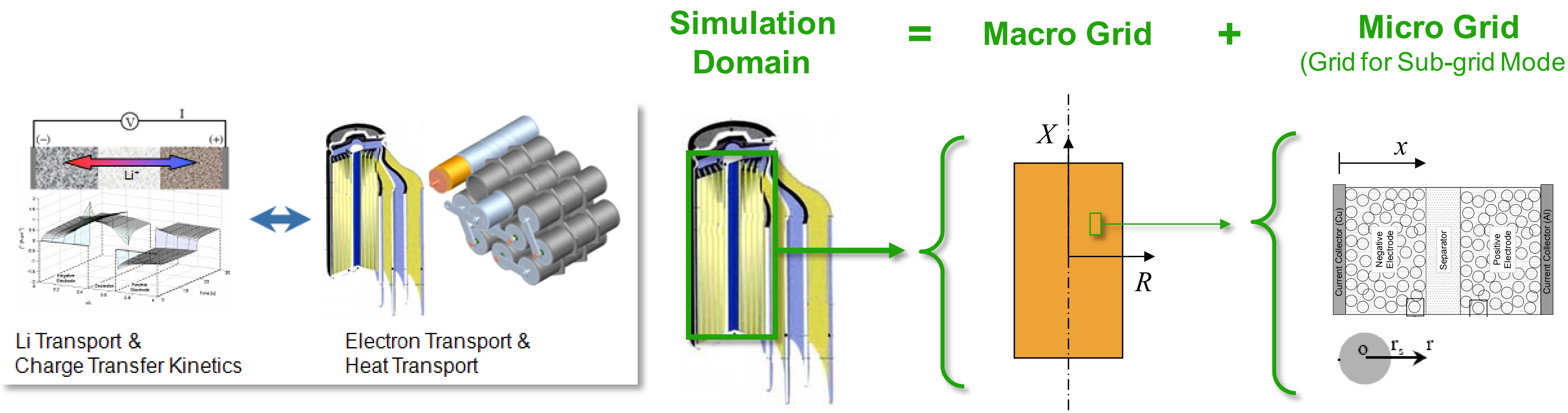


Electron Transport &
Heat Transport

Simply *Work?*
Extend model domain size up to cell scale to capture macroscopic design features, while maintaining model resolution to capture Li diffusion dynamics in electrode level scale ***???*** → *huge computational complexity and cost*

Approach

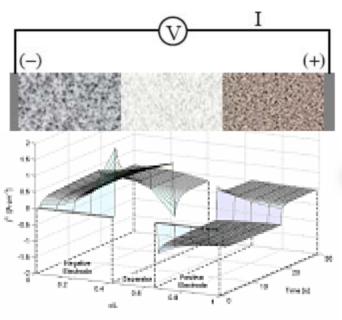
Multi-Scale Multi-Dimensional (MSMD) Model



- Captures macroscopic electron/heat transports, electrode scale Li diffusion dynamics/charge transfer kinetics in separate domains
- Physically couple the solution variables defined in each domain using multi-scale modeling schemes
- Runs in tolerable calculation time, practical for battery and system engineering design

Present Study

"Poorly designed electron and heat transport paths can cause excessive spatial ***non-uniformity in battery physics****, and then* *<u>deteriorate the performance</u>* *and* *<u>shorten the life</u>* *of the battery."*



Li Transport &
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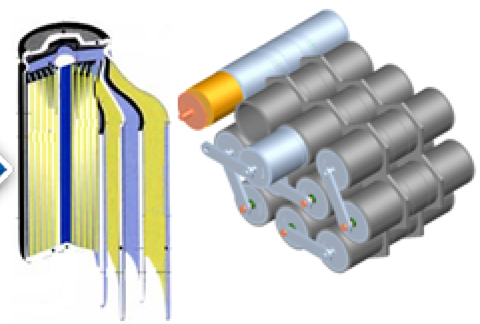


Electron Transport &
Heat Transport

Fixed Microscopic Designs ***Macroscopic Features as Design Variables***

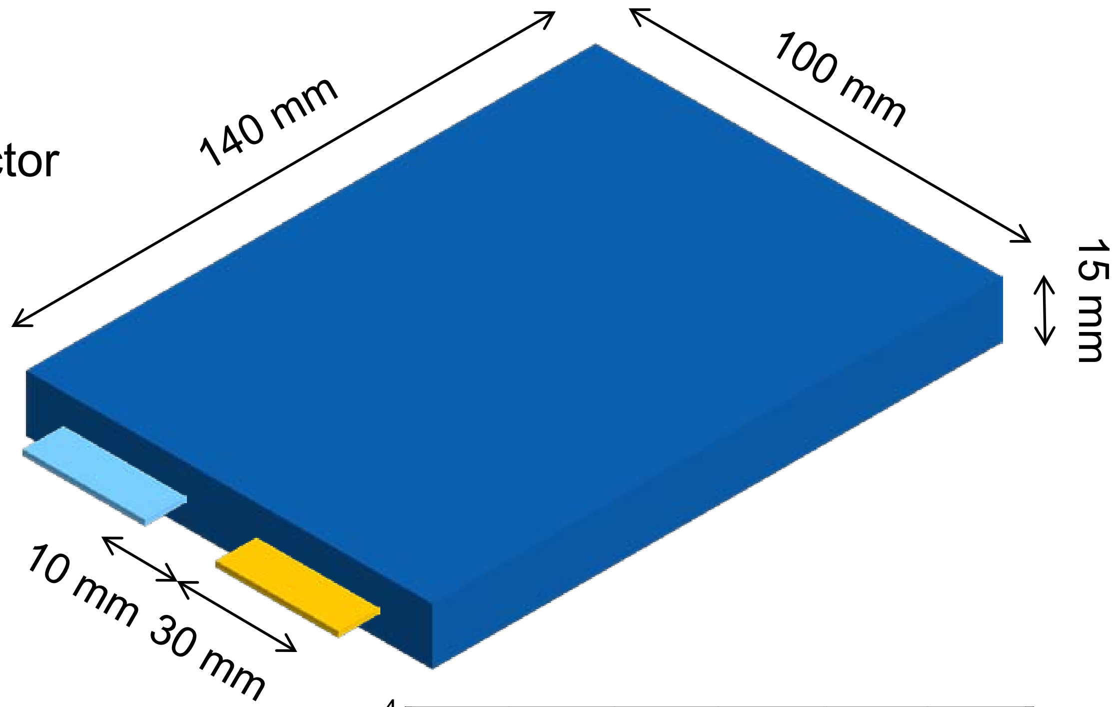
Objectives

Demonstrate the impact of macroscopic design factors on battery …

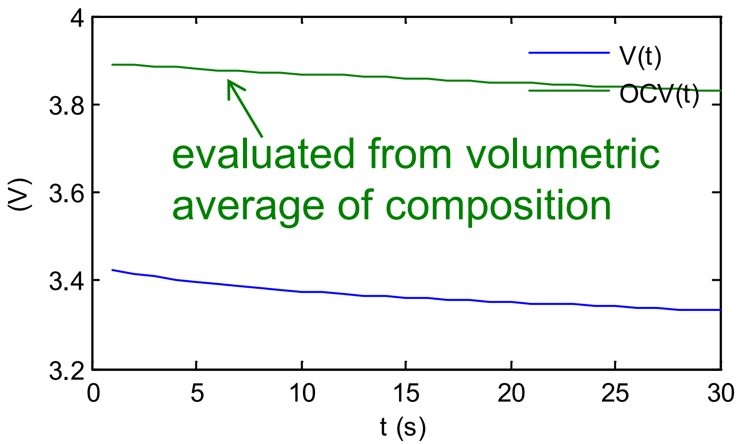
- Performance : *B2 abs# 252* (Kim & Smith) → This talk
- Life: *B2 abs# 255* (Smith & Kim)

Nominal Design – 10C discharge for 30 sec

- ✓ Stacked prismatic design
- ✓ 140 x 100 x 15 mm^3 form factor
- ✓ Tabs on a same side
- ✓ 20 Ah
- ✓ PHEV10 application

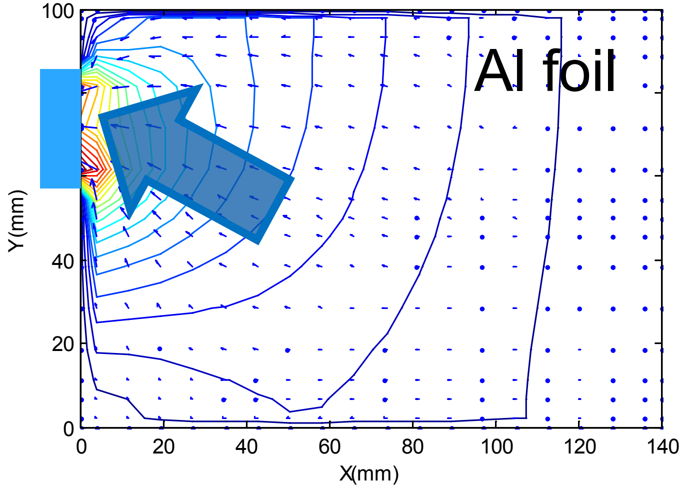


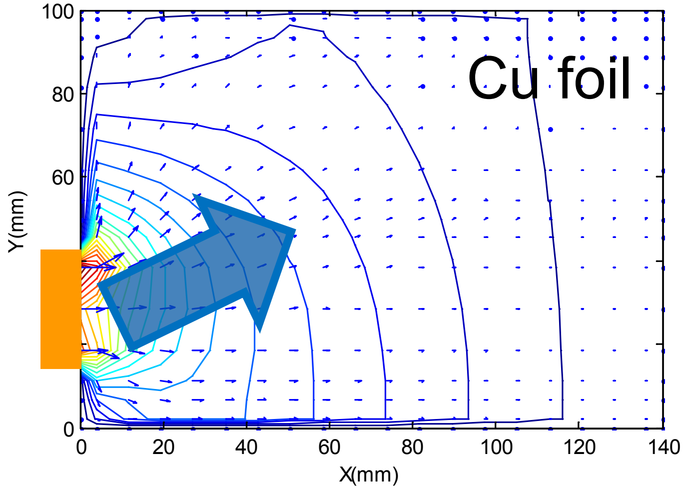
- ✓ 10C constant current discharge
- ✓ soc_{ini} = 90%
- ✓ Surface and tab cooling
- ✓ h_{inf} = 20 W/m^2K
- ✓ T_{amb} = 30°C
- ✓ T_{ini} = 30°C



Electrical Response – 10C Discharge

Current density field at metal collector foils after 30 sec discharge at mid-plane





Working potential between electrode planes after 30 sec discharge at mid-plane

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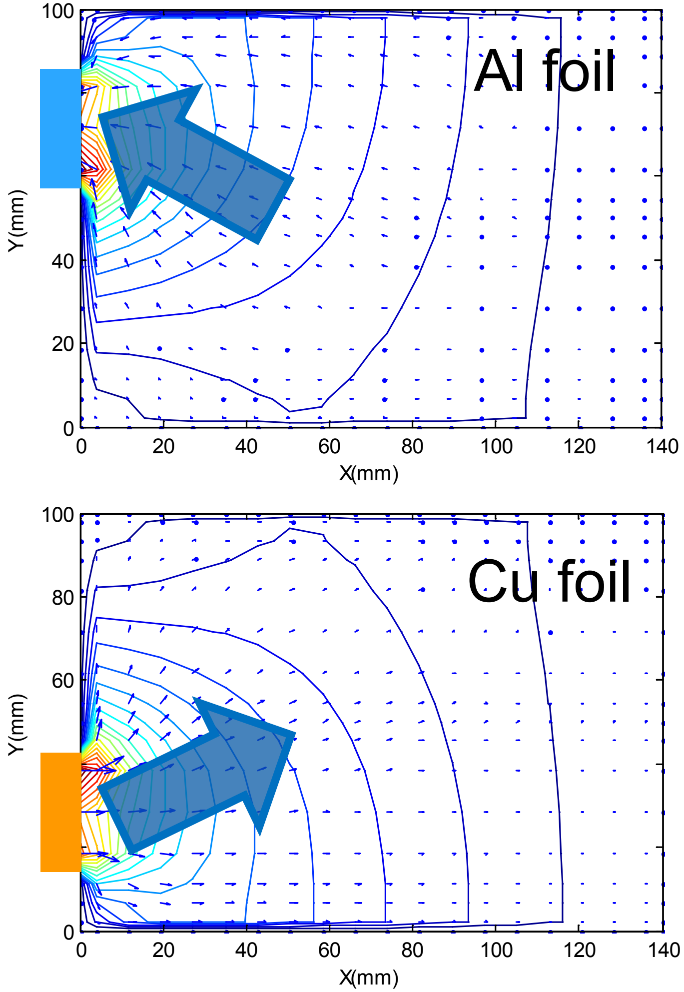

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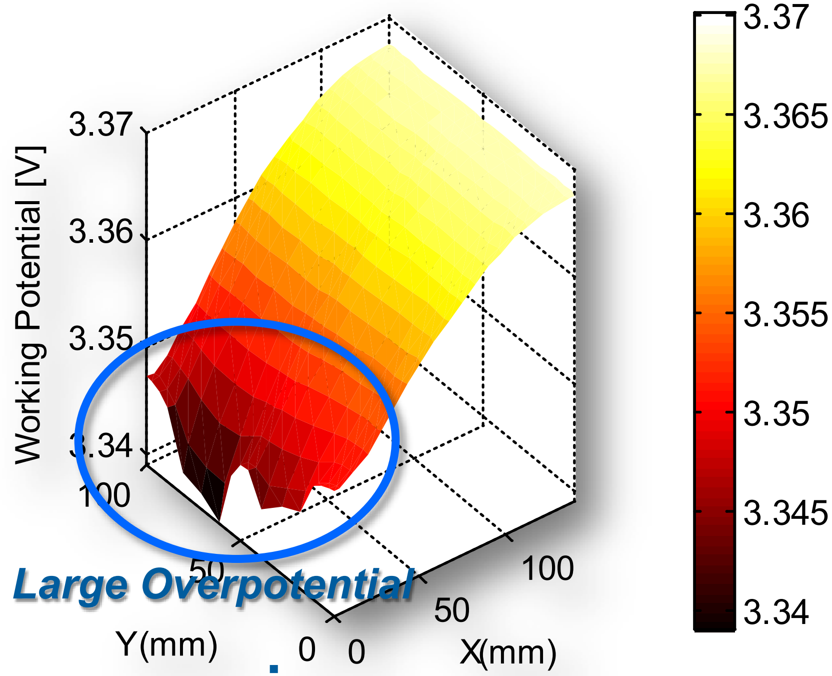
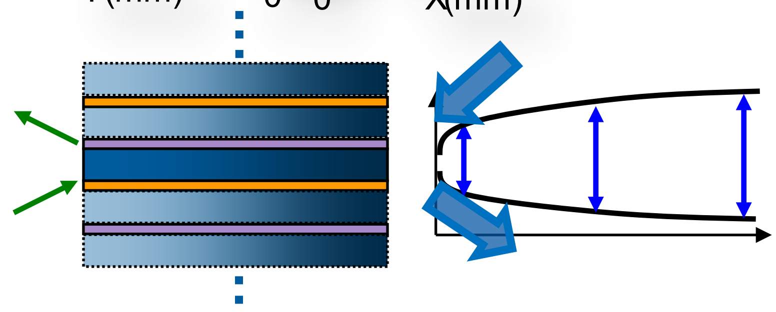
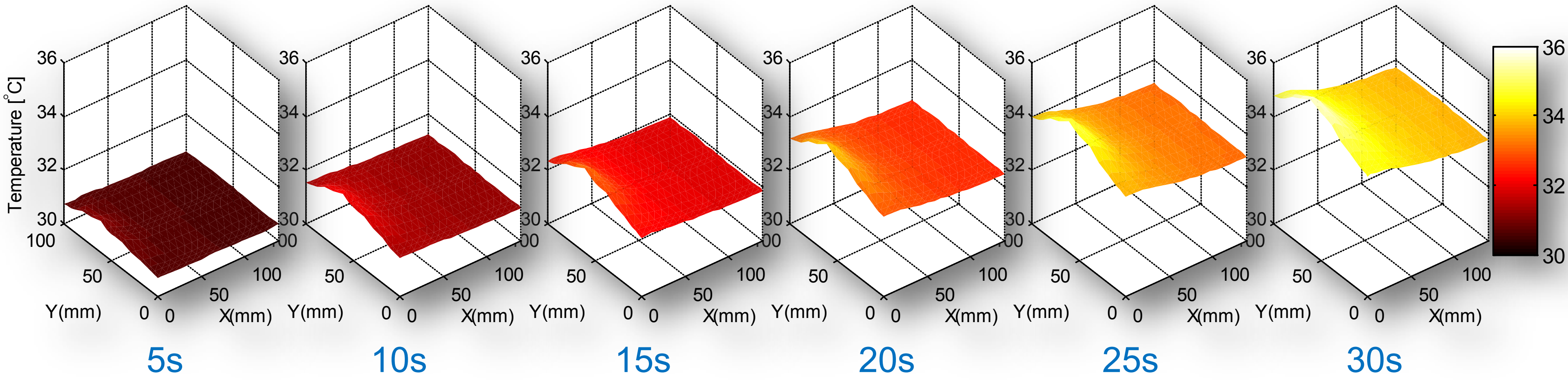
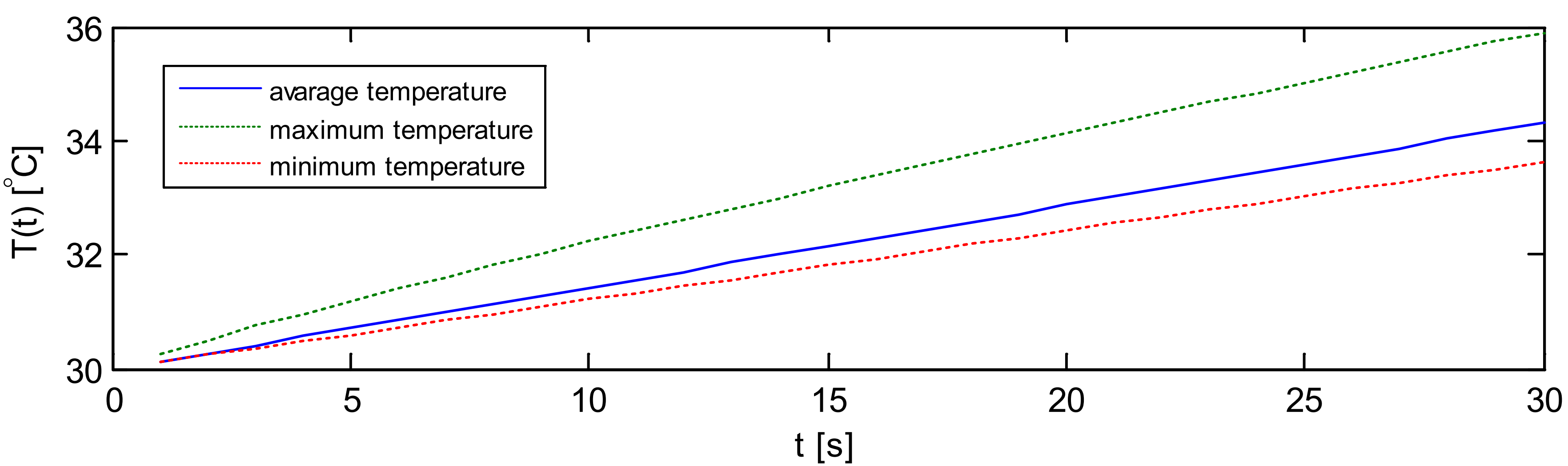




Thermal Response – 10C Discharge

Temperature Evolution at Mid-Plane

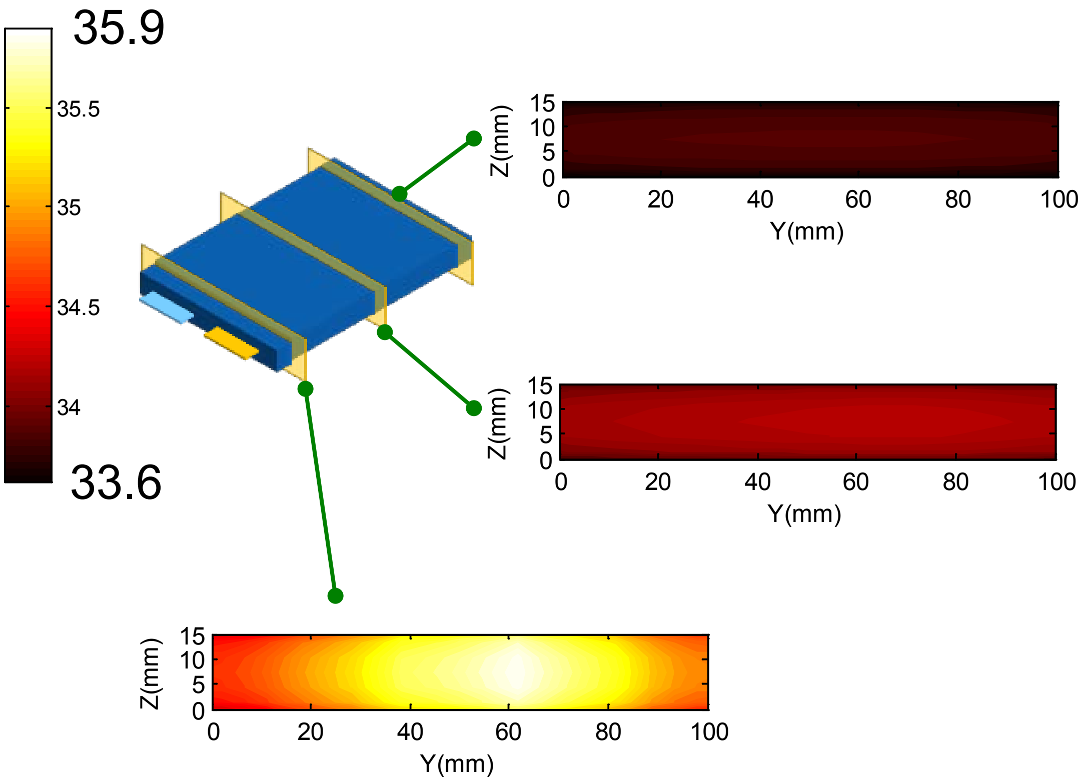


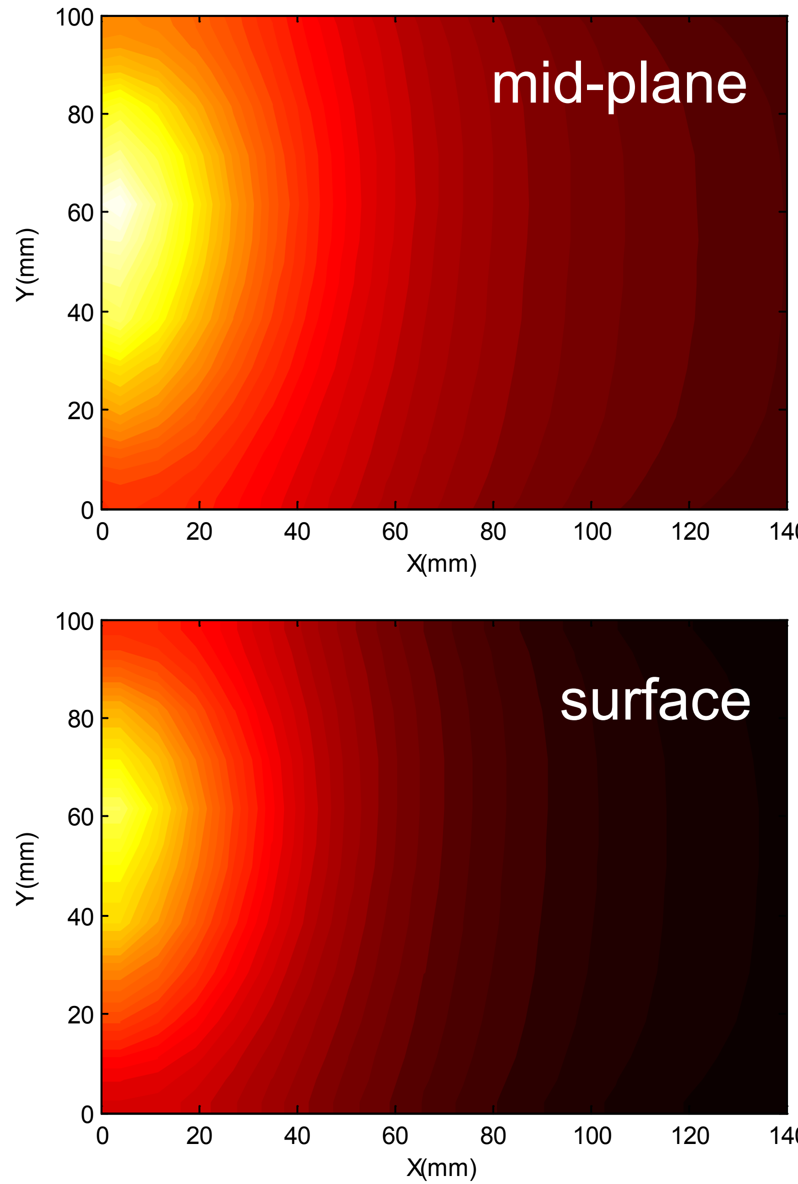


Thermal Response – 10C Discharge

Temperatures after 30 sec discharge

- ✓ T_{ini} =30.0 °C
- ✓ T_{avg}=34.3 °C
- ✓ ΔT=2.3 °C

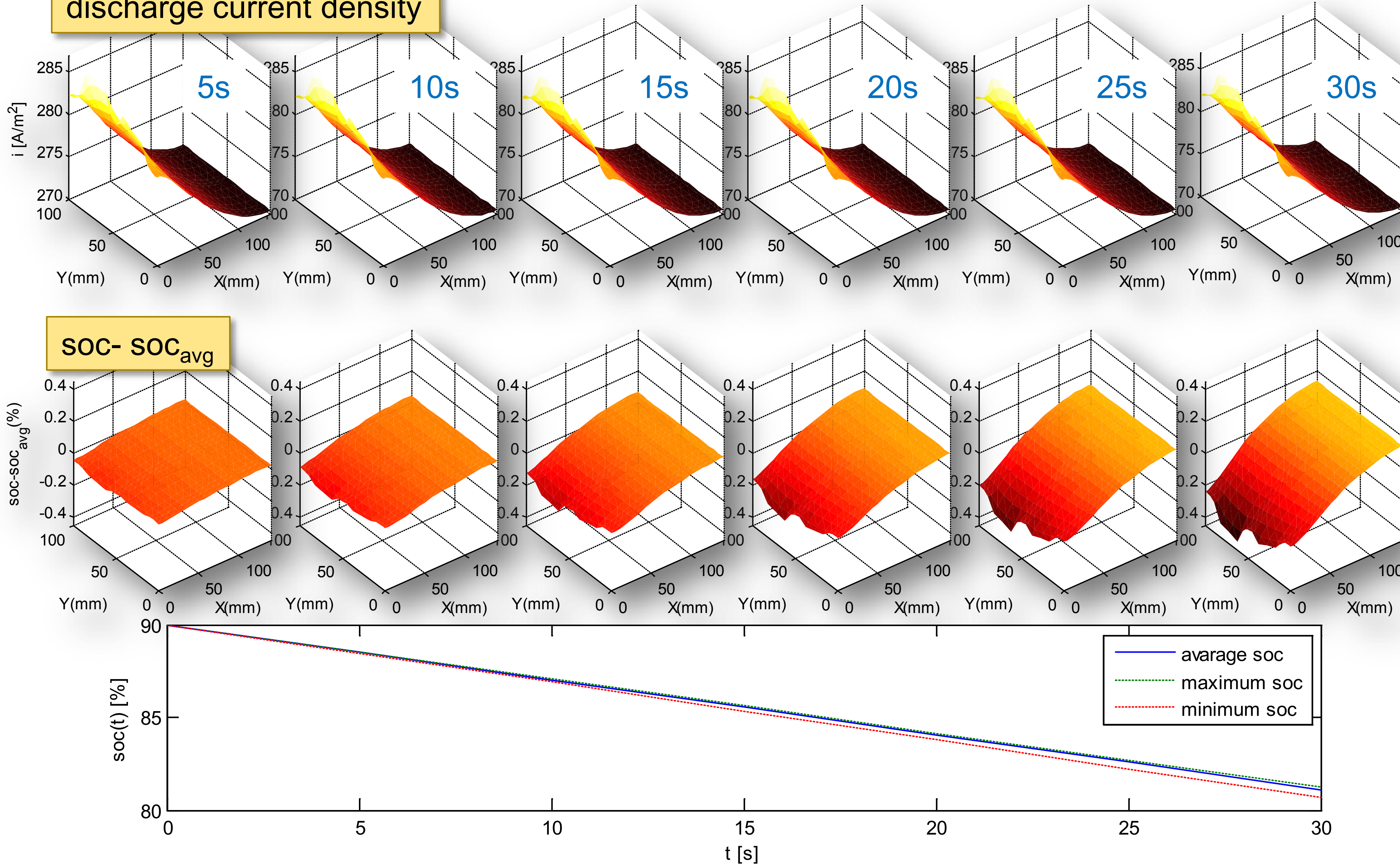




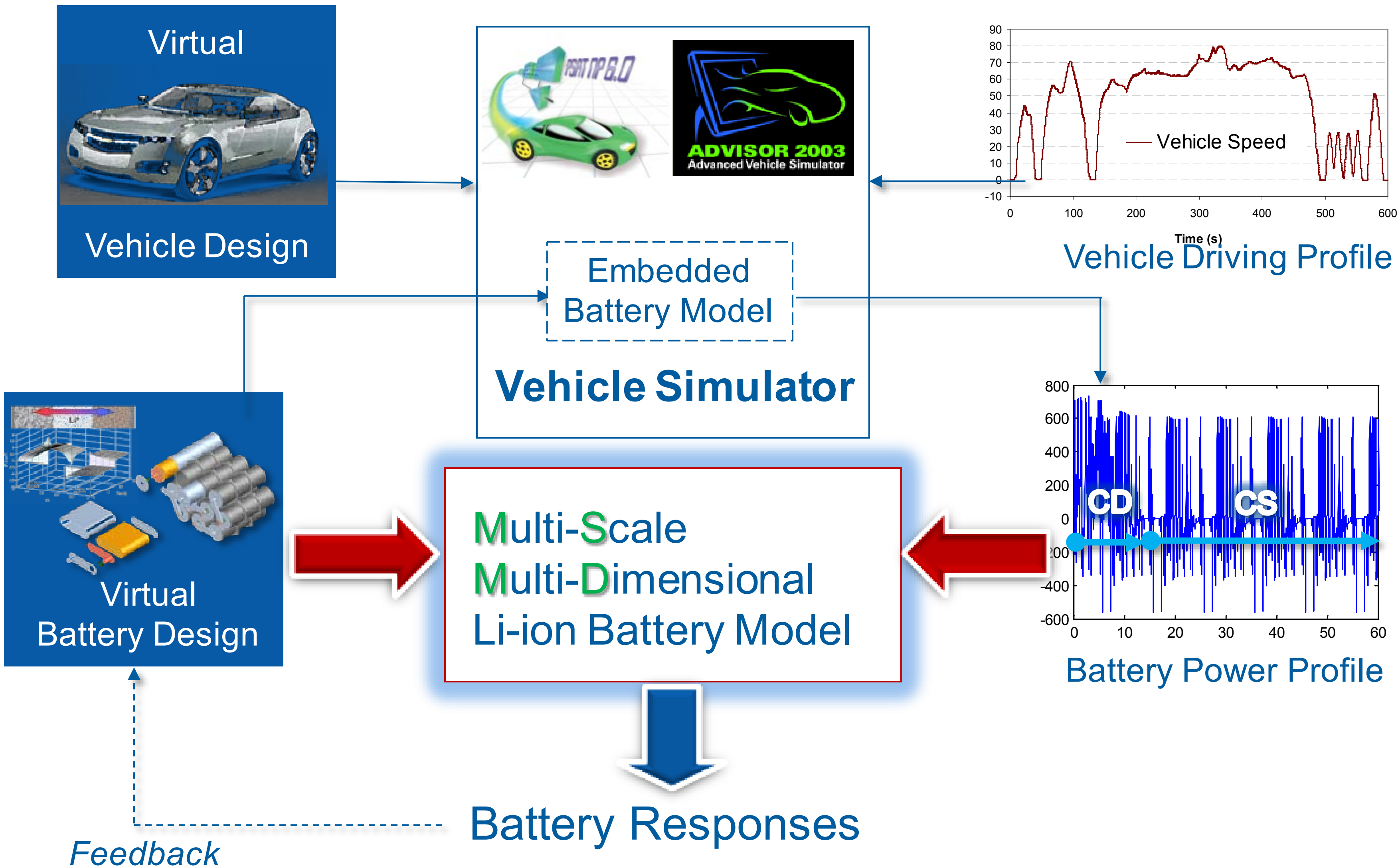
Electrochemical Response – 10C discharge

discharge current density

soc- soc_{avg}

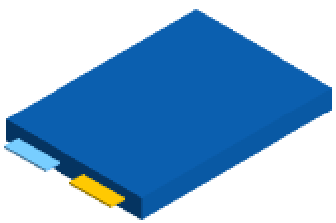


Virtual Design Evaluation



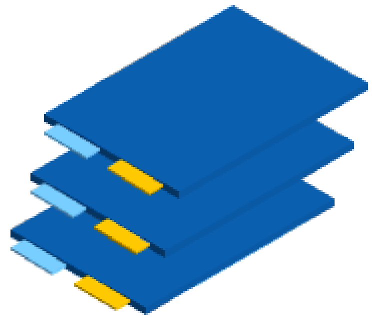
Alternative Cell Designs

Nominal Design



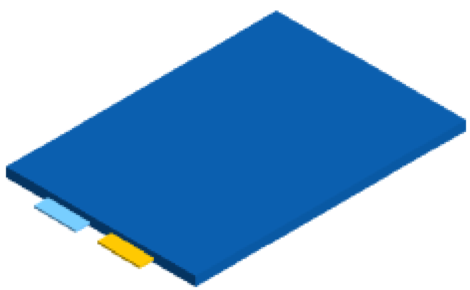
- 140 x 100 x 15 mm^3
- Tabs on a same side
- 20 Ah

Small Capacity SC



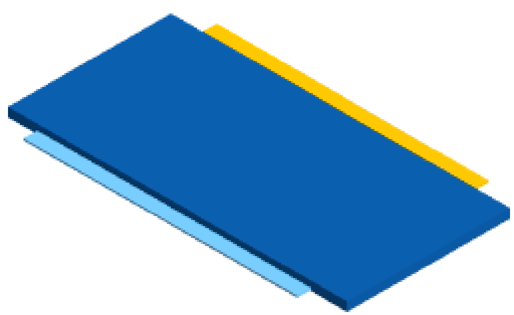
- 3 x (140 x 100 x 5) mm^3
- Same tab design
- 3 x 6.67 Ah
- Same electrode area/stack layer
- 1/3 thickness
- ~ 3x surface area

Thin and Wide *TW*



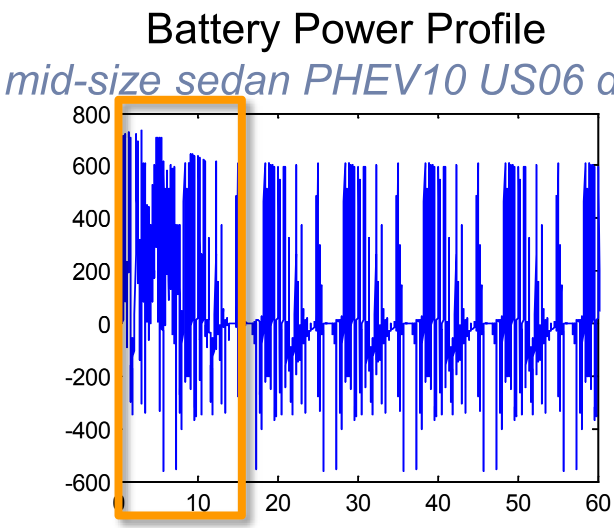
- 200 x 140 x 7.5 mm^3
- Same tabs
- 20 Ah
- 2x electrode area/stack layer
- 1/2 thickness
- ~ 2x surface area

Counter Tab *CT*

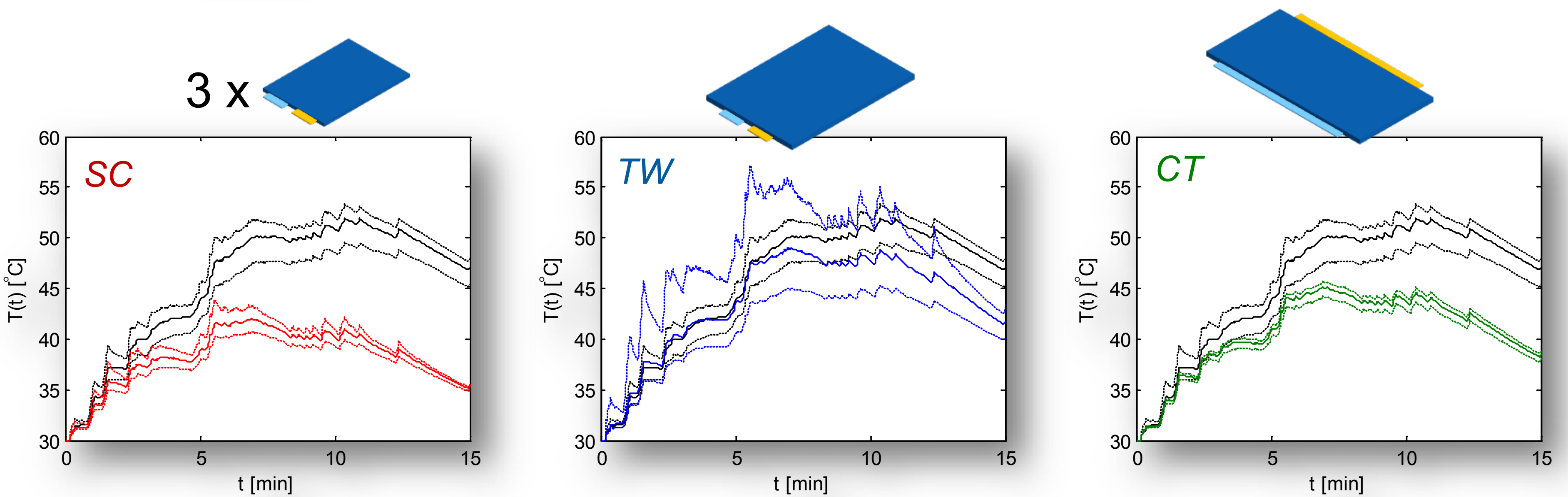


- 250 x 120 x 7 mm^3
- Wide-counter tab design
- 20 Ah
- ~2x electrode area/stack layer
- ~1/2 thickness
- ~2x surface area

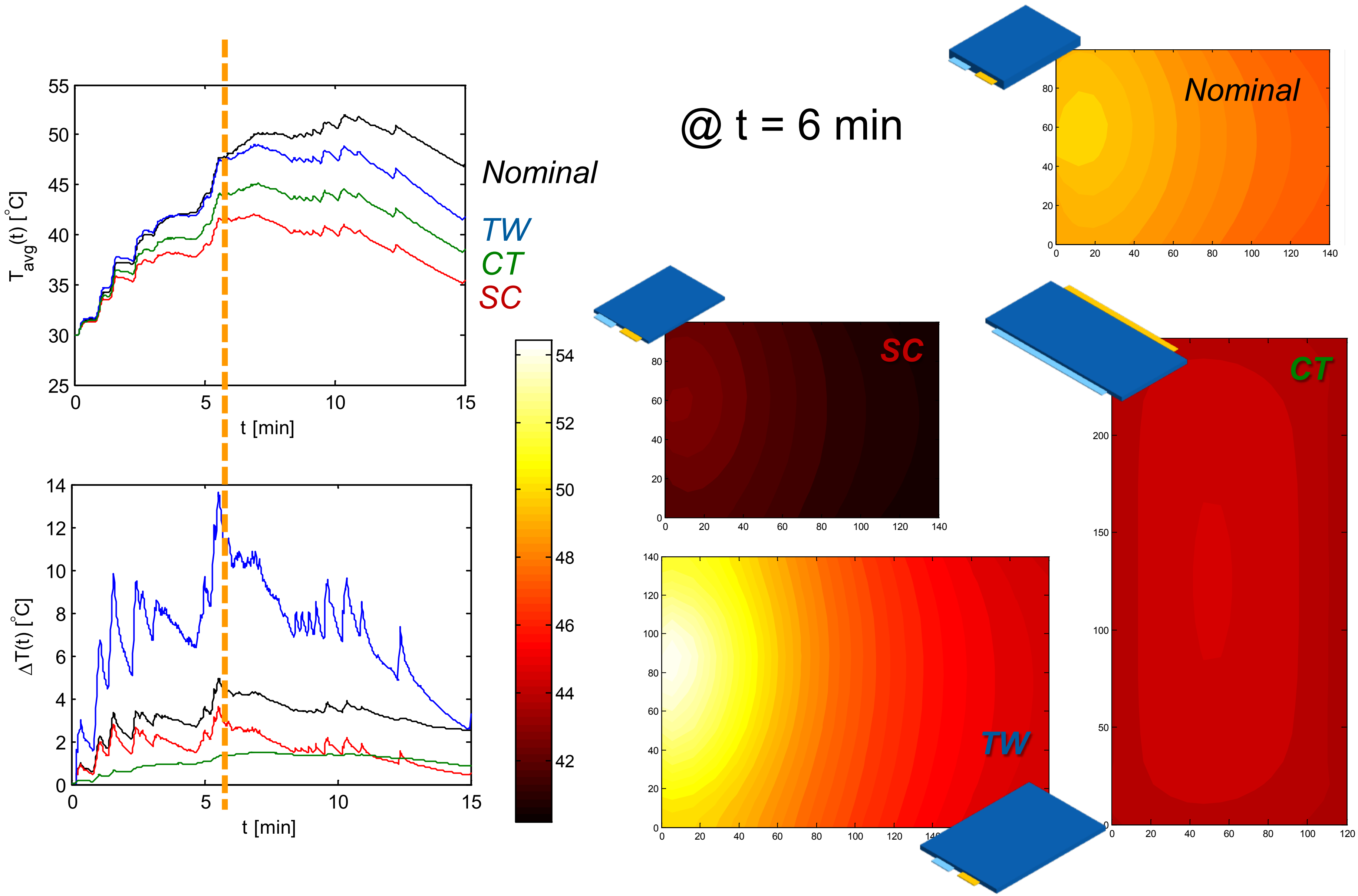
Thermal Behavior Comparison



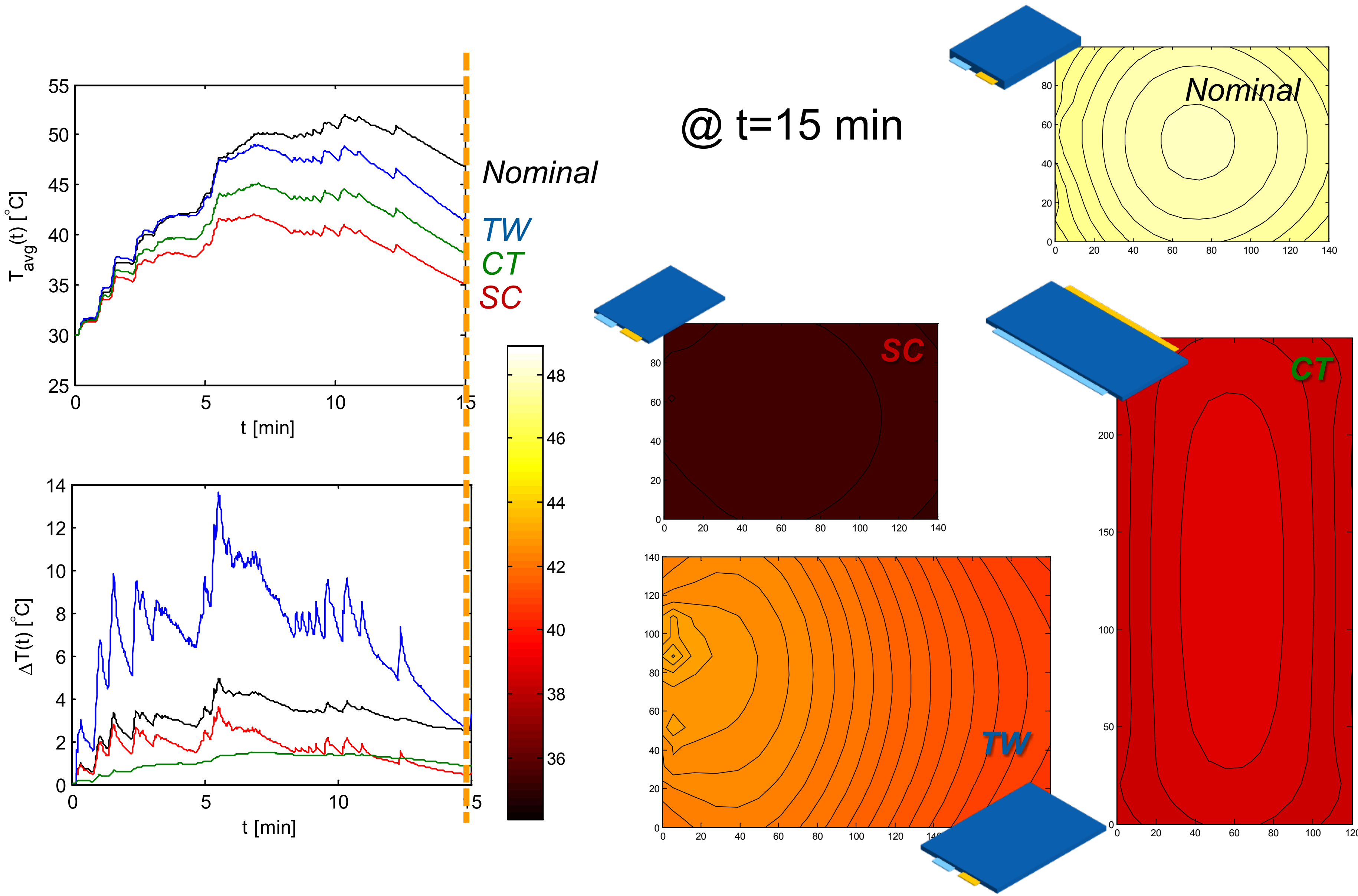
- 15-minute drive (CD + CS)
- soc_{ini} = 90%
- Surface and tab cooling
- h_{inf} = 20 W/m²K
- T_{amb} = 30°C
- T_{ini} = 30°C



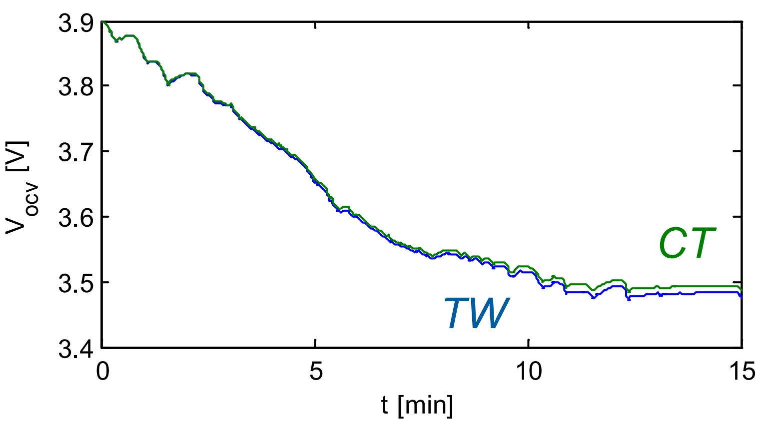
Temperature Imbalance during CD Drive

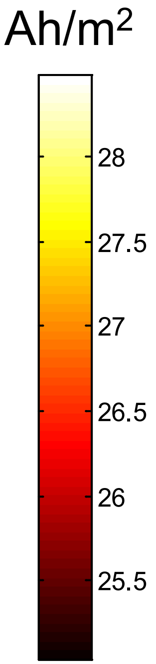


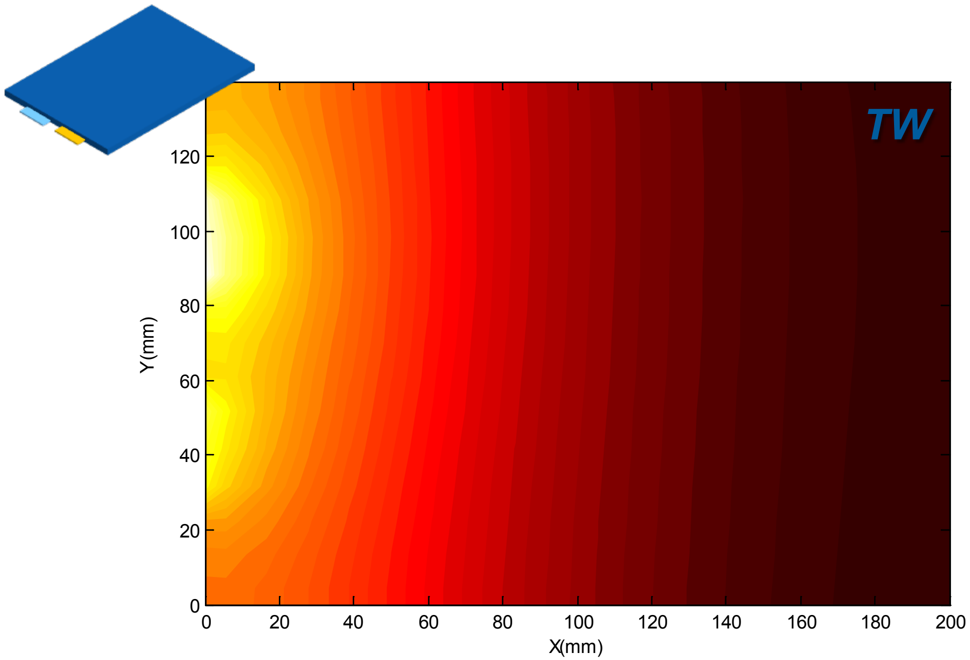
Temperature Imbalance during CS drive

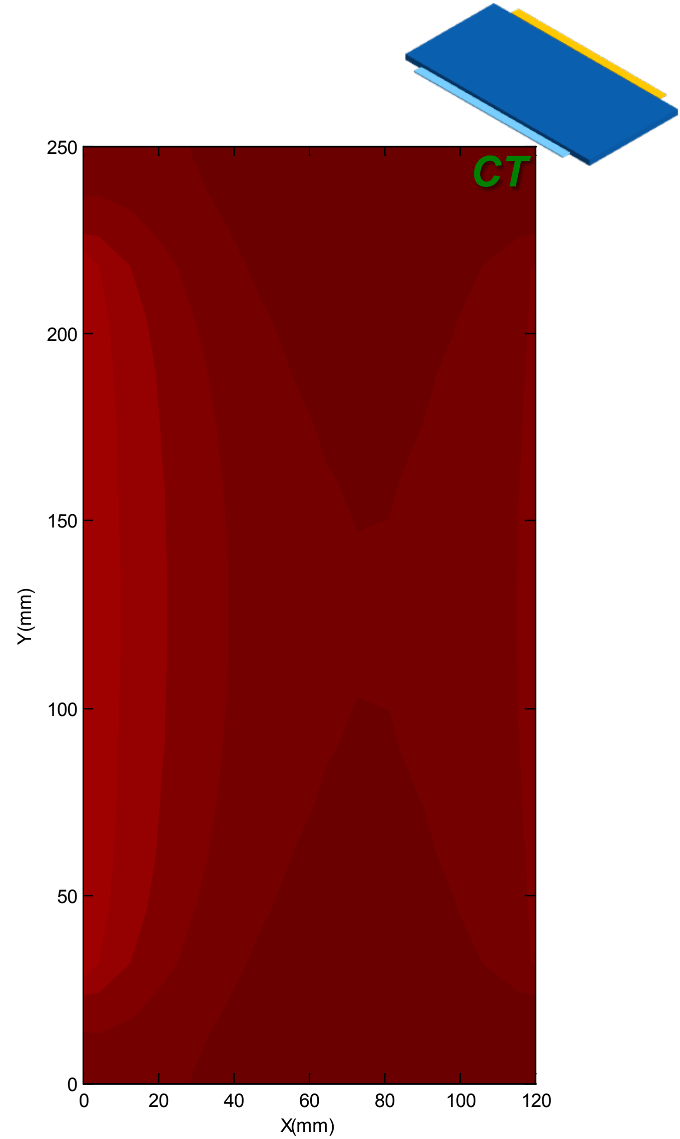


Ah Throughput Imbalance *TW* vs *CT*









Summary

- Nonuniform battery physics, which is more probable in large-format cells, can cause unexpected performance and life degradations in lithium-ion batteries.
- A Multi-Scale Multi-Dimensional model was used for evaluating large format prismatic automotive cell designs by integrating micro-scale electrochemical process and macro-scale transports.
- Thin form factor prismatic cell with wide counter tab design would be preferable to manage cell internal heat and electron current transport, and consequently to achieve uniform electrochemical kinetics over a system.

- Engineering questions to be addressed in *further discussion* include …

What is the optimum form-factor and size of a cell?
Where are good locations for tabs or current collectors?
How different are externally proved temperature and electric signals from non-measurable cell internal values?
Where is the effective place for cooling? What should the heat-rejection rate be?

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