NREL National Renewable Energy Laboratory
Innovation for Our Energy Future

Multi-Scale Multi-Dimensional Li-ion Battery Model for Better Design and Management

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PRiME PACIFIC RIM MEETING ON ELECTROCHEMICAL AND SOLID-STATE SCIENCE

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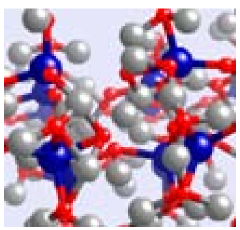
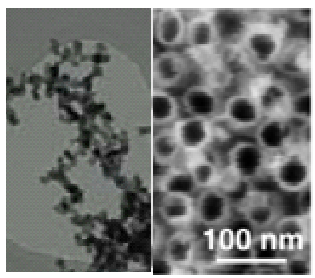
Multi-Scale Physics in Li-Ion Battery

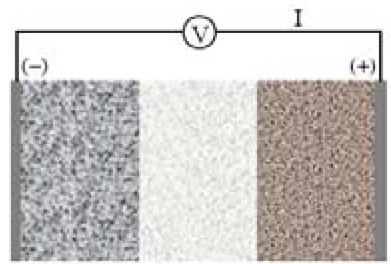
Requirements & Resolutions

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

Performance
Life
Cost
Safety





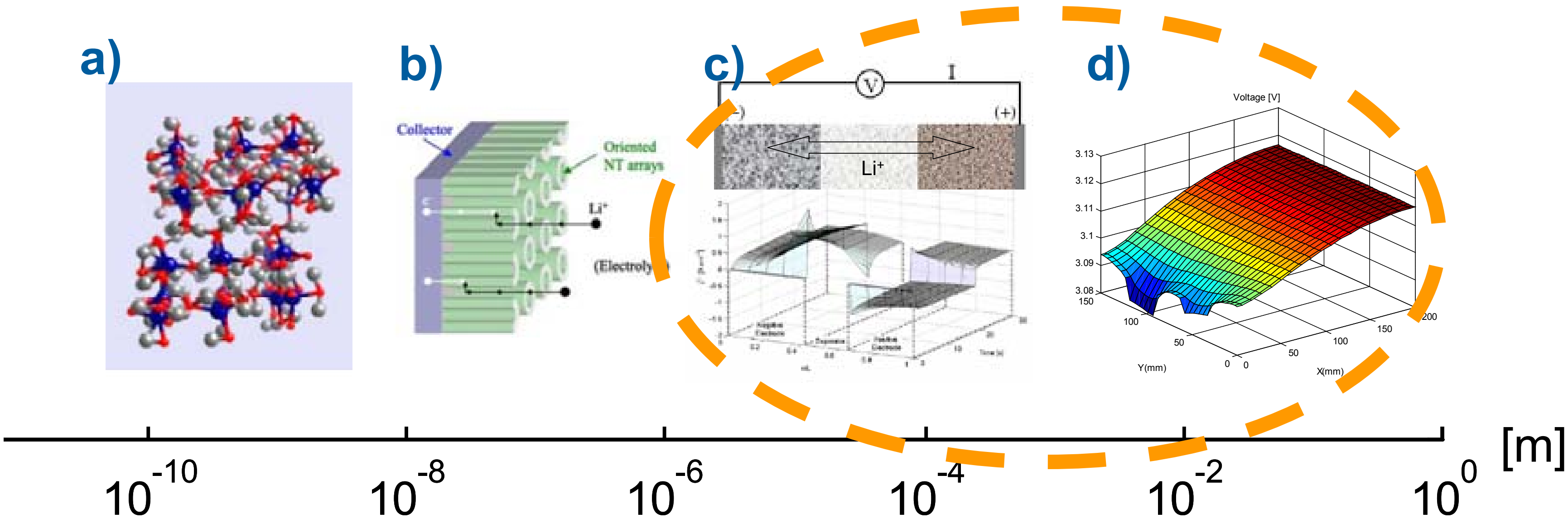


10^{-10} 10^{-8} 10^{-6} 10^{-4} 10^{-2} 10^{0} [m]

Design of Materials	Design of Electrode Architecture	Design of Electrodes Pairing and Lithium Transport	Design of Electron Current & Heat Transport
Voltage *Capacity* *Lattice stability* *Kinetic barrier* *Transport property*	*Li transport path (local)* *Electrode surface area* *Deformation & fatigue* *Structural stability* *Surface physics*	*Electrodes selection* *Li transport* *Porosity, tortuosity* *Layer thicknesses* *Load conditions*	*Electric & thermal connections* *Dimensions, form factor* *Component shapes*

The Need for a Multi-Scale Model

Numerical approaches focusing on different length scale physics



a) Quantum mechanical and molecular dynamic modeling
b) Numerical modeling for addressing the impacts of the architecture of electrode materials
c) 1D performance model capturing solid-state and electrolyte diffusion dynamics
d) Cell-dimension 3D model for evaluating macroscopic design factors

Why Macro-scale Transport Becomes Critical

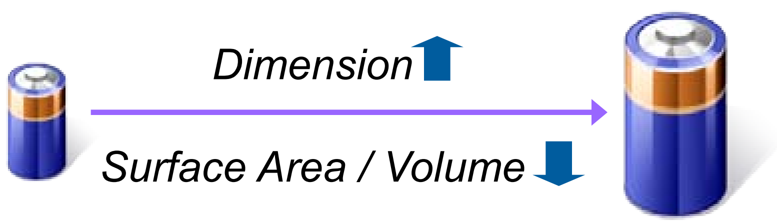
Sub-electrode scale physics
Kinetics
Li diffusion
Ion transport
Heat dissipation

Design of current and heat flow paths

Spatial variation of …

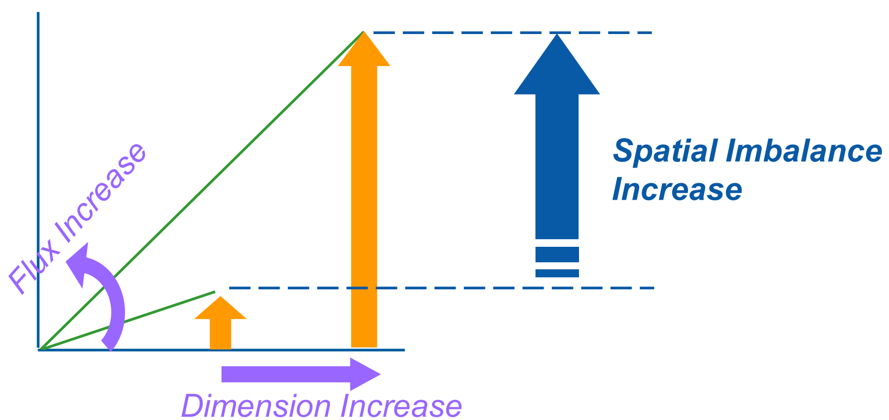
- Electric potentials
- Temperatures

Size Effect



Flux (gradient) ↑
Barrier (distance) ↑

Spatial Difference ↑↑
(gradient x distance)



Approach in the Present Study

Multi-Scale Multi-Dimensional (MSMD) Modeling

To address ...

- Multi-scale physics from sub-micro-scale to battery-dimension-scales
- Difficulties in resolving microlayer structures in a computational grid

Simulation Domain = **Macro Grid** + **Micro Grid** (Grid for Sub-grid Model)

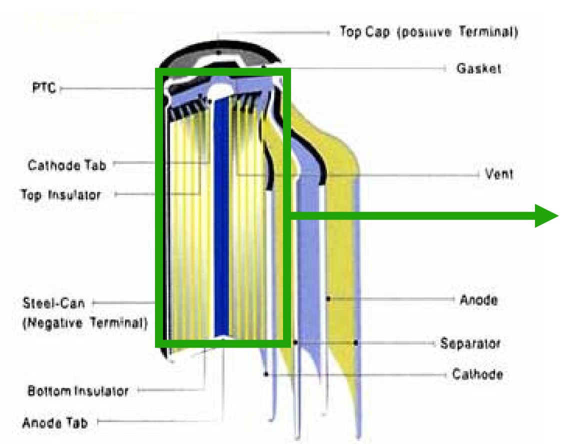
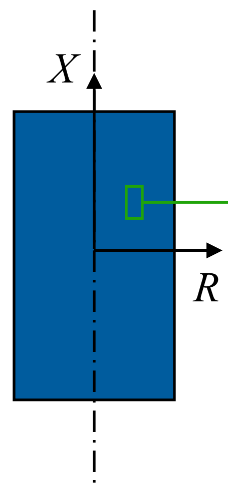
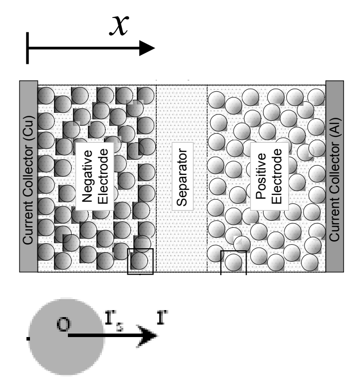


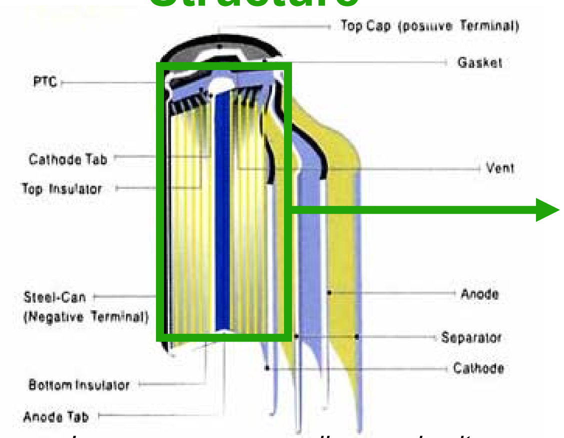
Image source: www.dimec.unisa.it





Solution Variables

Detailed Structure ≈ **Cell Dimension Transport Model** + **Electrode Scale Submodel (1D)**



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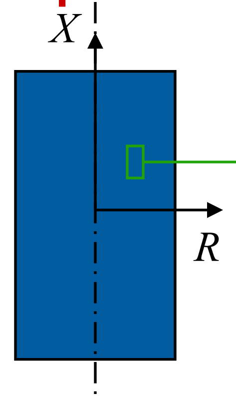
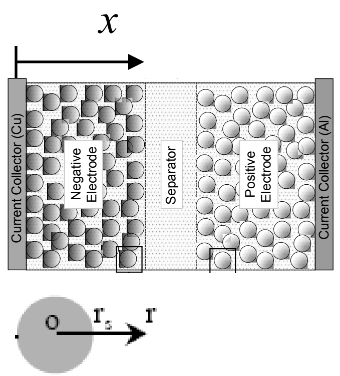




$$T(X,R,t)$$
$$V(X,R,t)$$
$$i(X,R,t)$$
$$SOC(X,R,t)$$
$$Q(X,R,t) = \int_x Q_i \frac{Adx}{V}$$

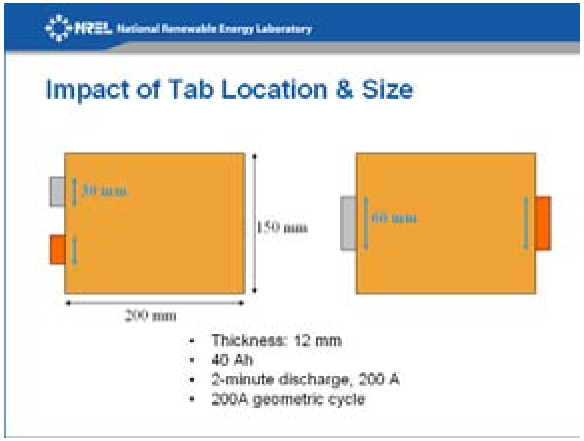
⟷

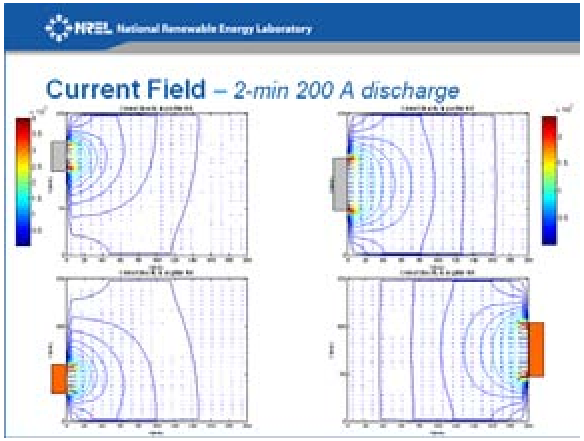
$$\phi_s(X,R,x,t)$$
$$\phi_e(X,R,x,t)$$
$$c_s(X,R,x,r,t)$$
$$c_e(X,R,x,t)$$
$$j_{Li}(X,R,x,t)$$
$$Q_i(X,R,x,t)$$

NOTE:
Selection of solution scheme for either grid system is independent of the other.

Previous Studies

AABC 08, Tampa, May 2008





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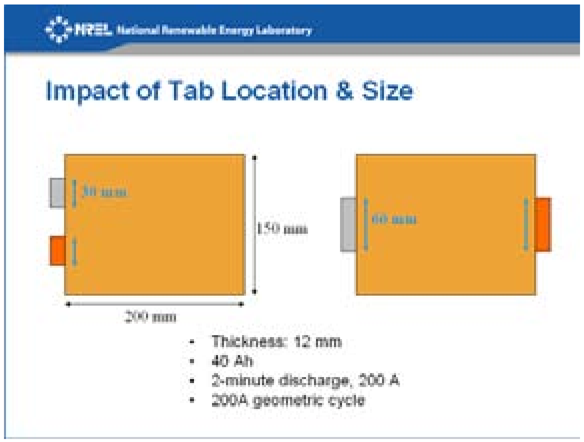

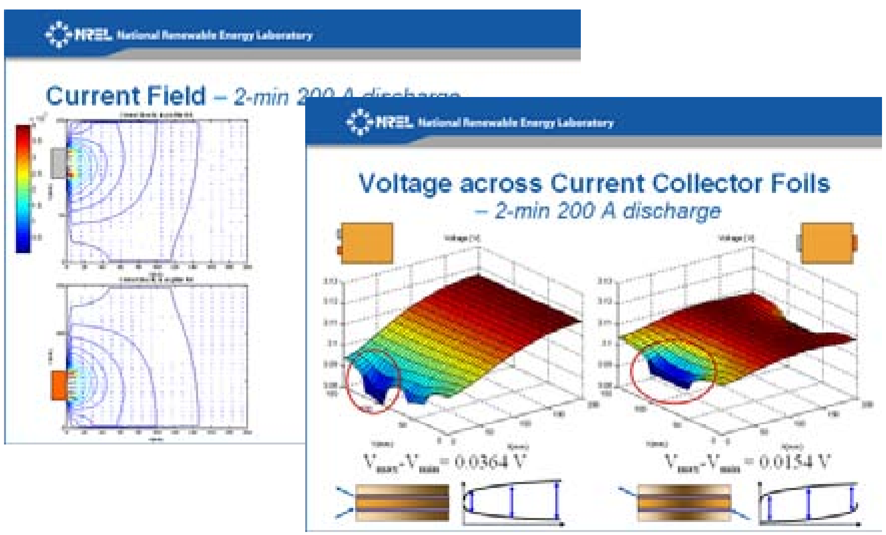

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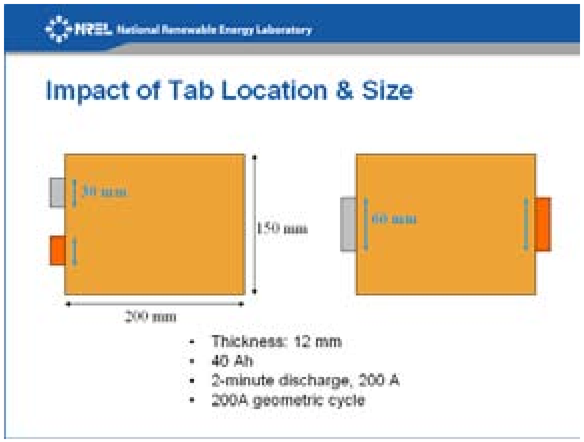

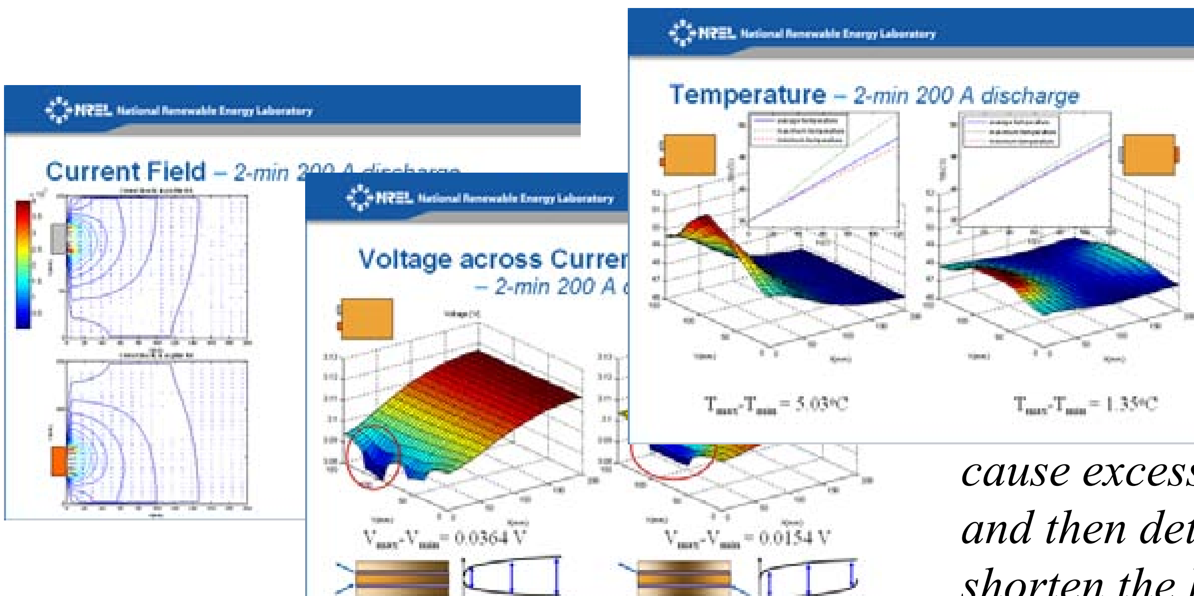

Findings:

"Poorly designed electron and heat transport paths can cause excessive nonuniform use of materials, and then deteriorate the performance and shorten the life of the battery."

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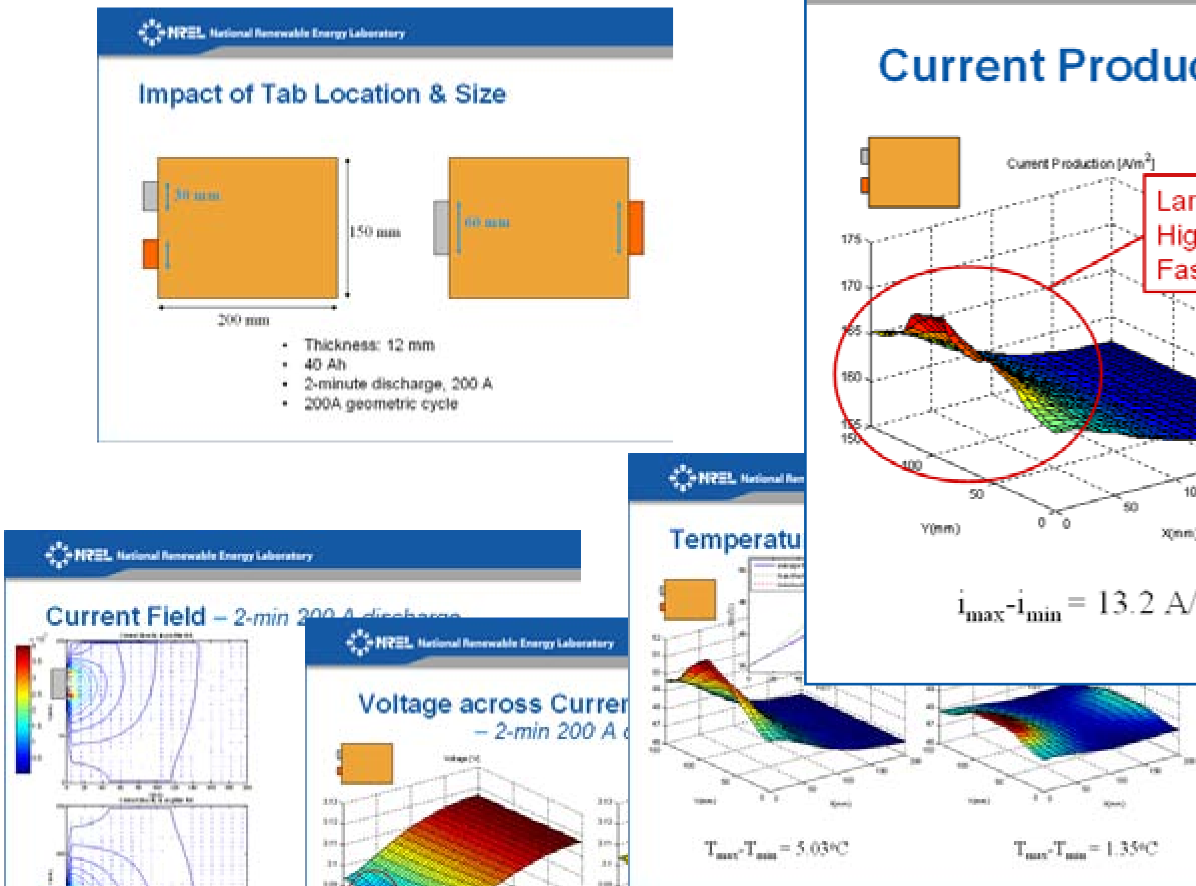

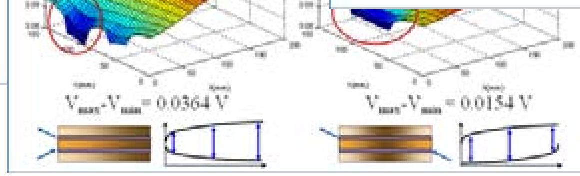

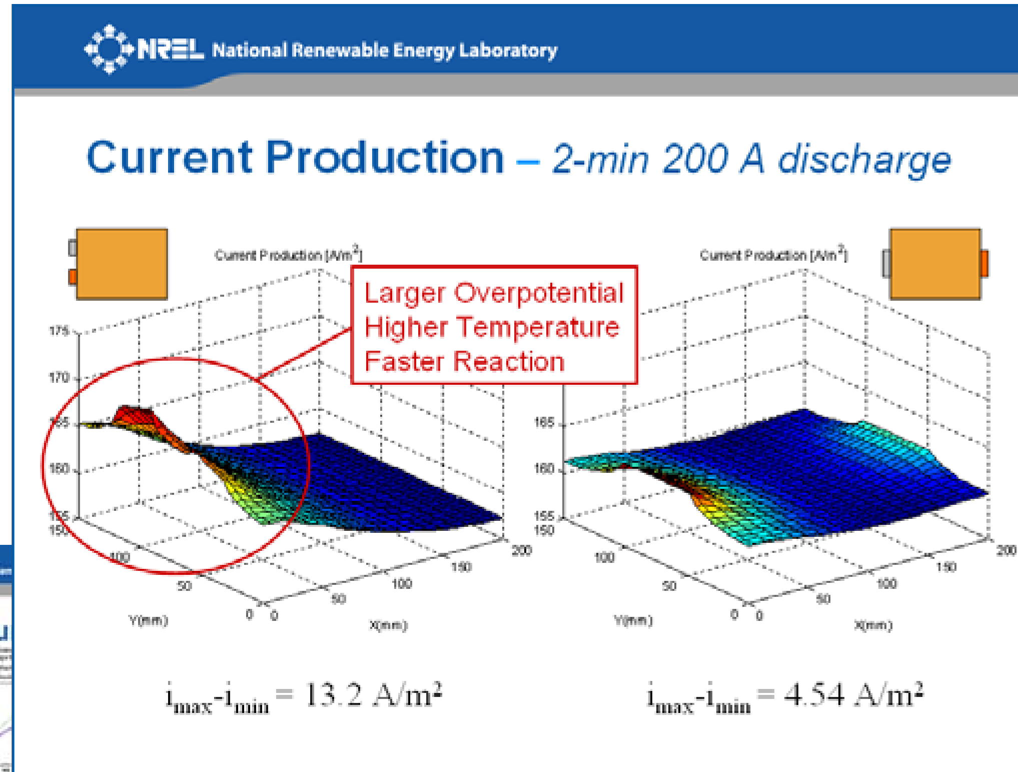

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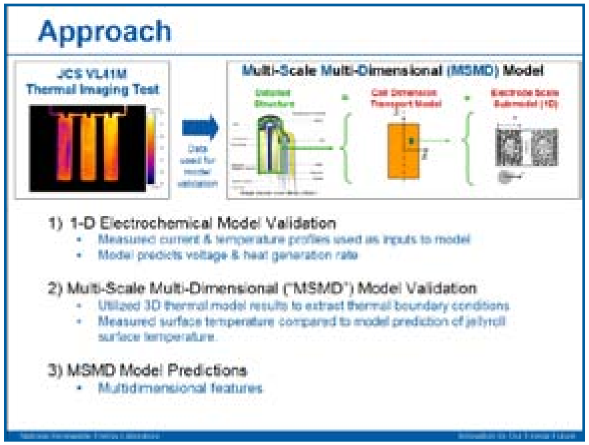
Model Validation Study against Thermal Imaging Test Data



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"Heat and electron transport interacts with micro-scale electrochemical processes and determines the distribution of temperature and electric potential."

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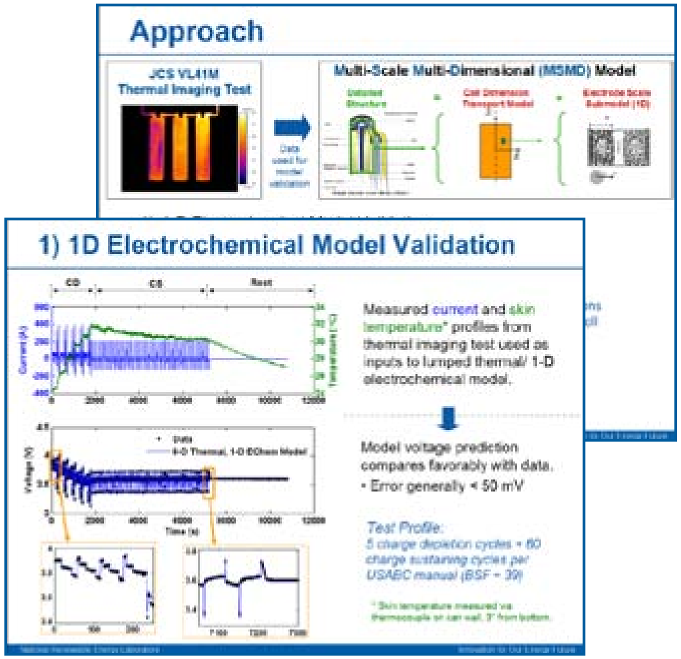

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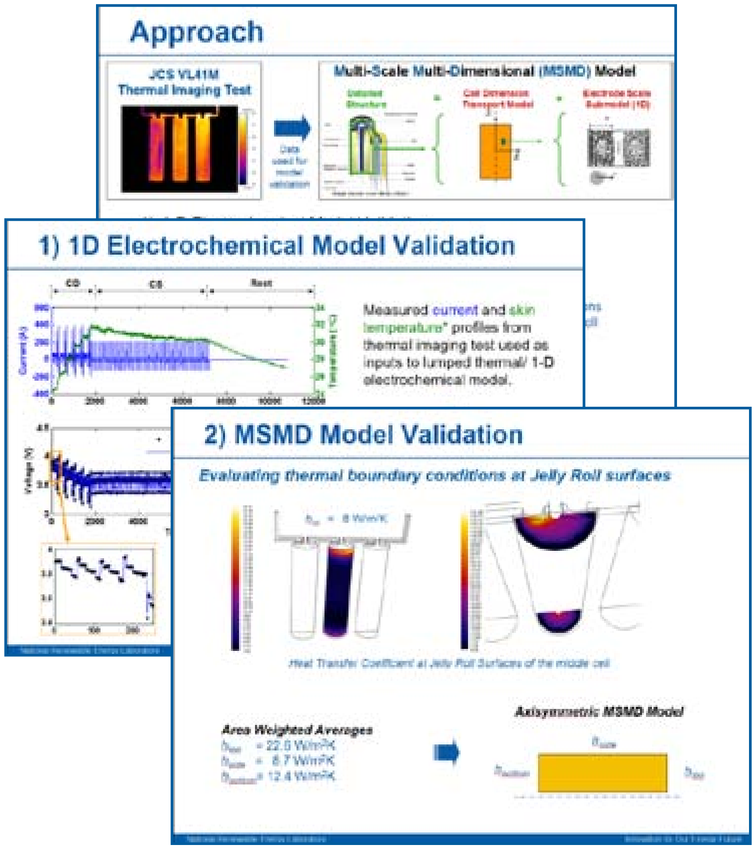

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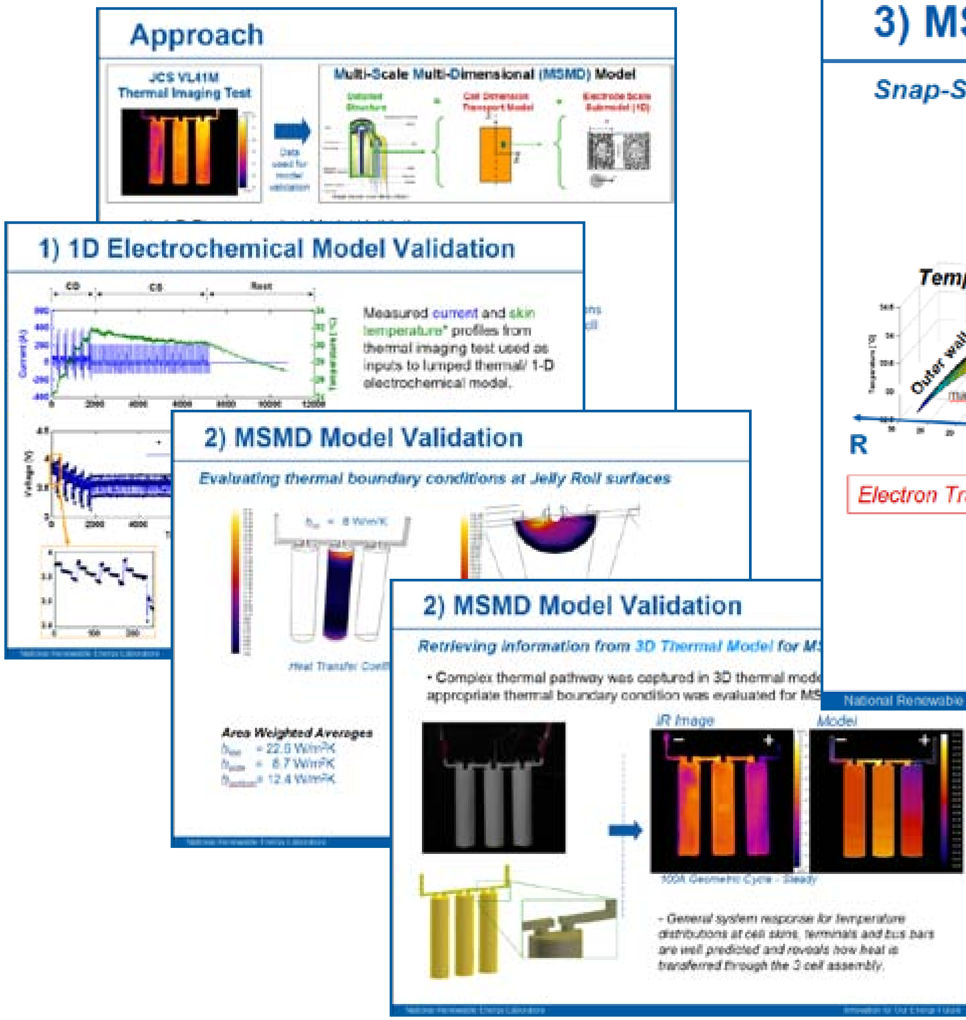

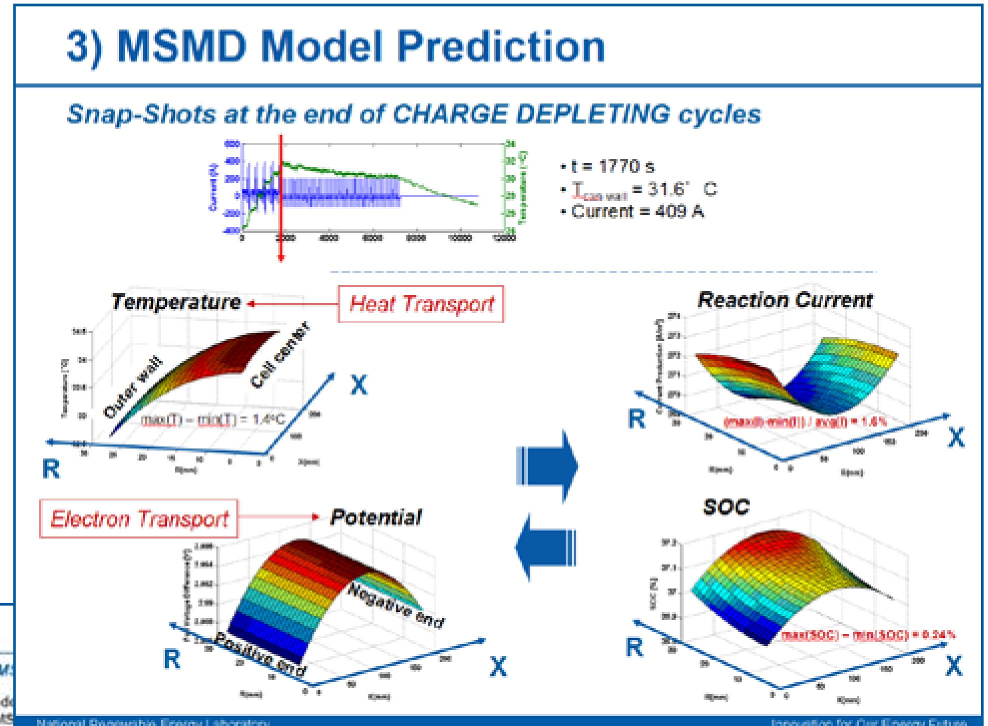

Findings:

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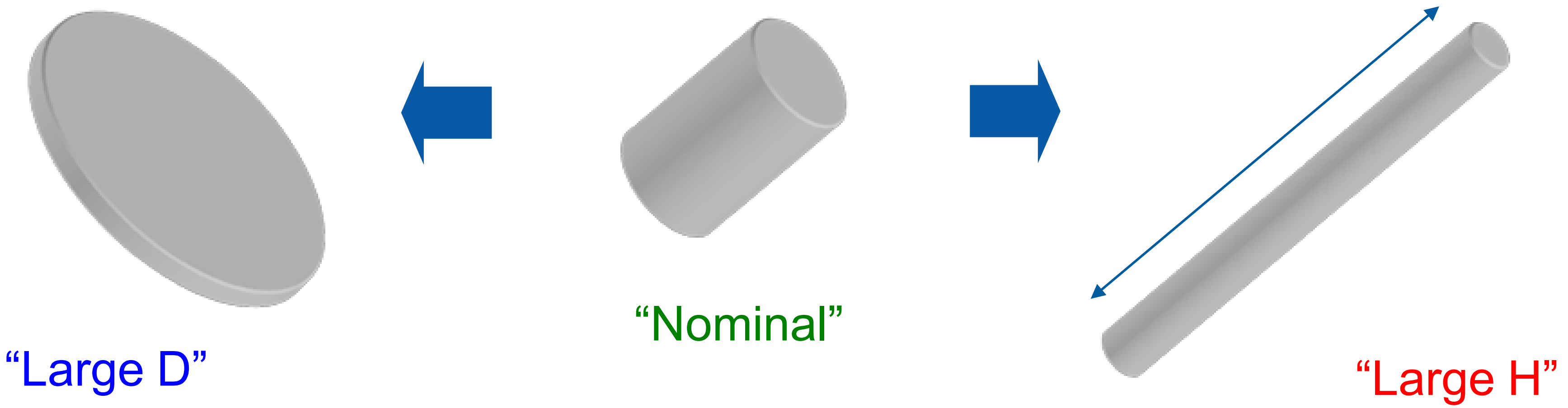
Current Analysis

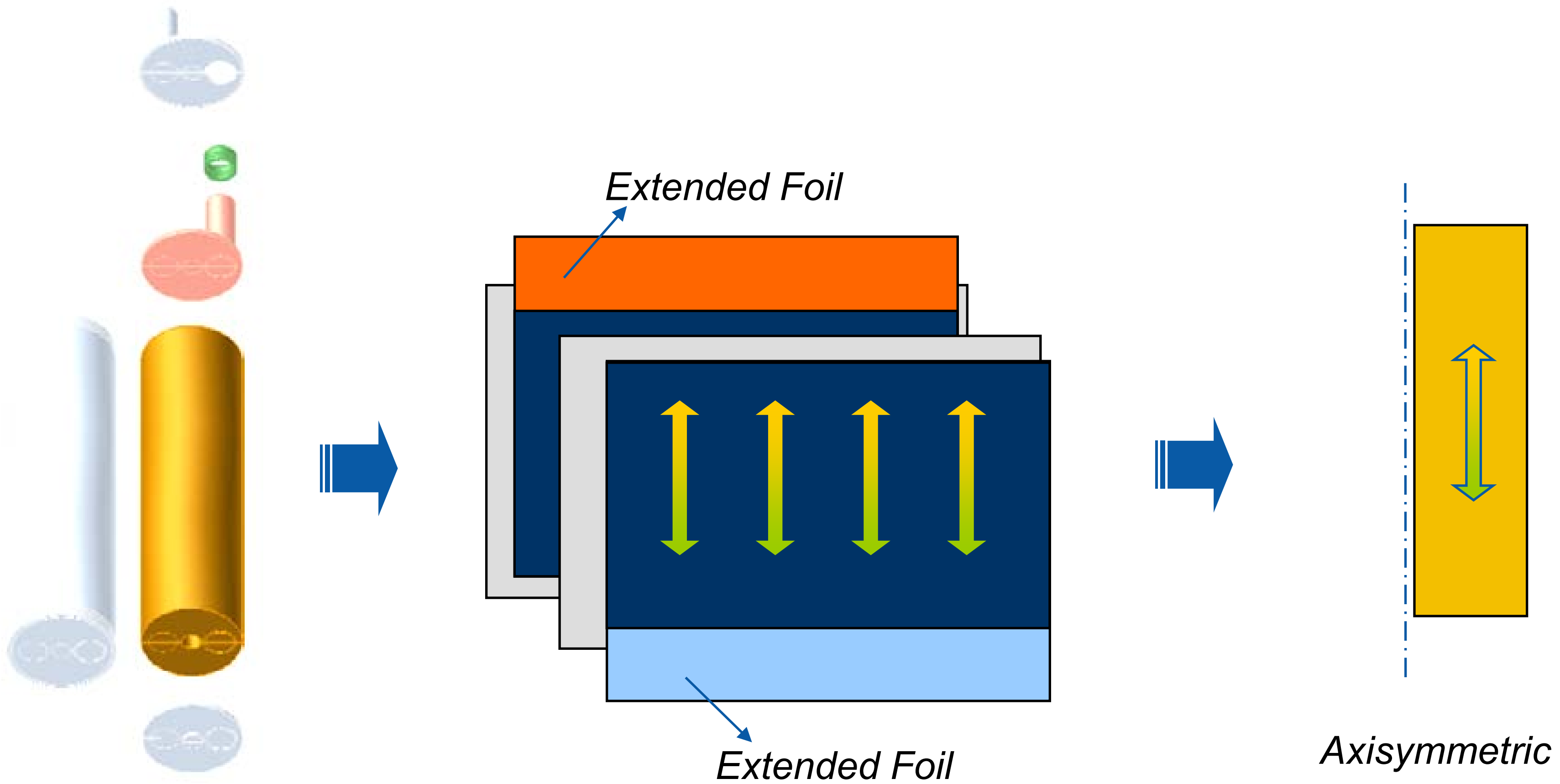
Macro-Scale Design Evaluation

Impacts of “Aspect Ratio” of a Cylindrical Cell

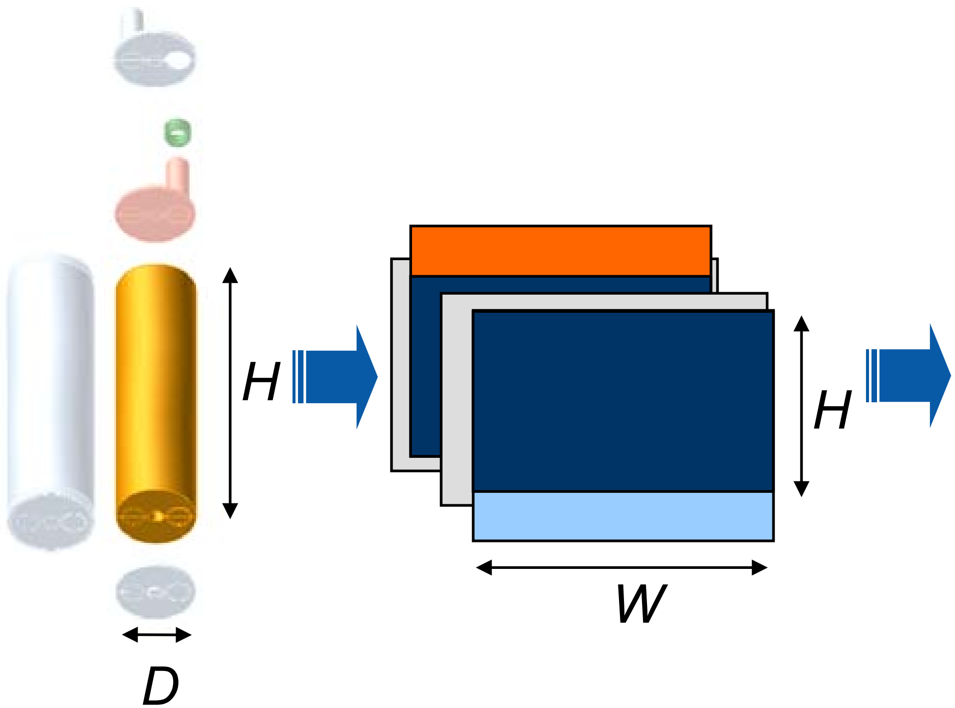


Each cell was virtually designed to deliver 20 Ah for PHEV-10 Applications.

Assumption for Model Simplification

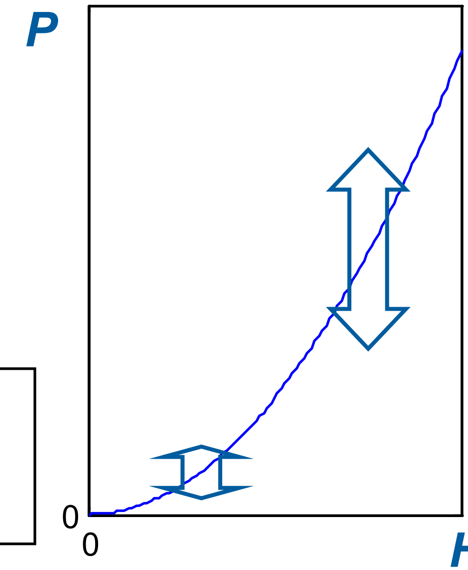


Brief Look at What "H/D Ratio" Means



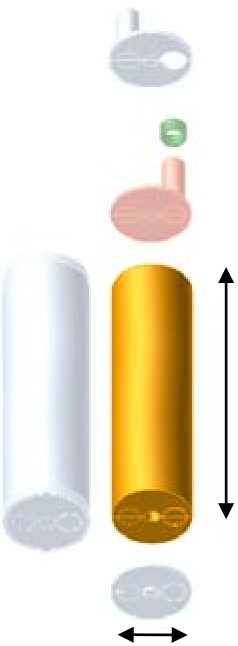
$$P_{loss,foil} \sim \frac{\rho \cdot i''^2}{\delta} H^2$$

i'': current [A/m^2]
ρ: resistivity
δ: foil thickness



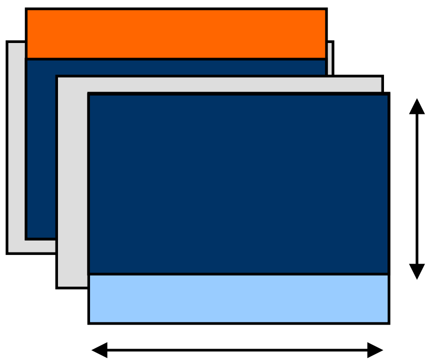
Volume = const
Identical electrodes → *H x W = const*
Same foil thicknesses
Al: 20 μm, Cu: 15 μm

Brief Look at What “H/D Ratio” Means



H

D



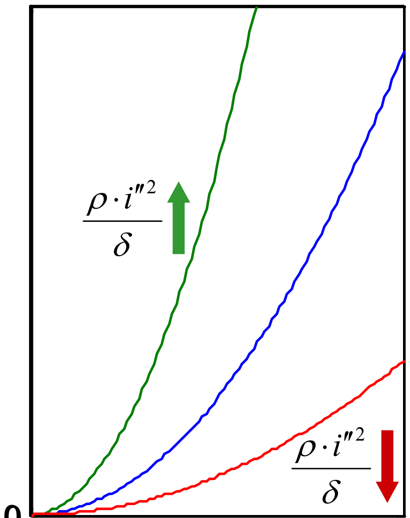
H

W

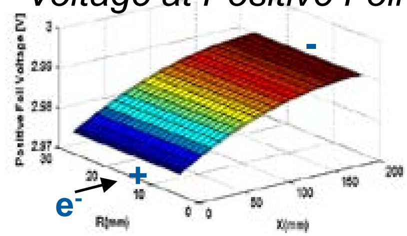
$$P_{loss,foil} \sim \frac{\rho \cdot i''^2}{\delta} H^2$$

$$\Delta V_{foil} \sim \frac{\rho \cdot i''}{\delta} H^2$$

i'': current [A/m^2]
ρ: resistivity
δ: foil thickness



Voltage at Positive Foil



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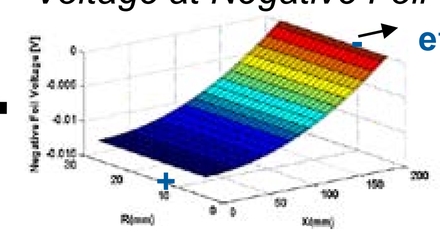
Voltage at Negative Foil



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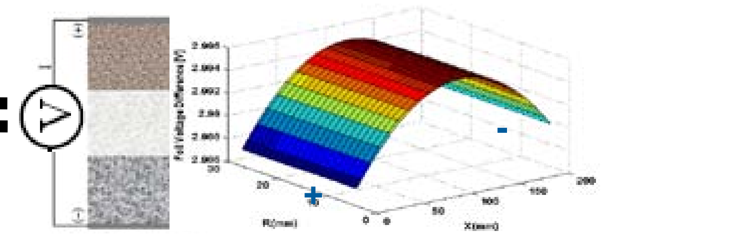


Volume = const
Identical electrodes
Same foil thicknesses
Al: 20 μm, Cu: 15 μm

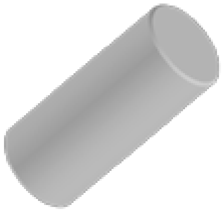
→ *H x W = const*

10-s Power Capability Comparison

Large H

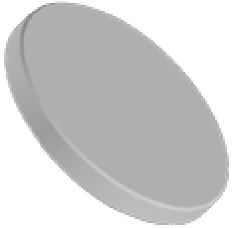
D[mm]: 28
H[mm]: 350

Nominal

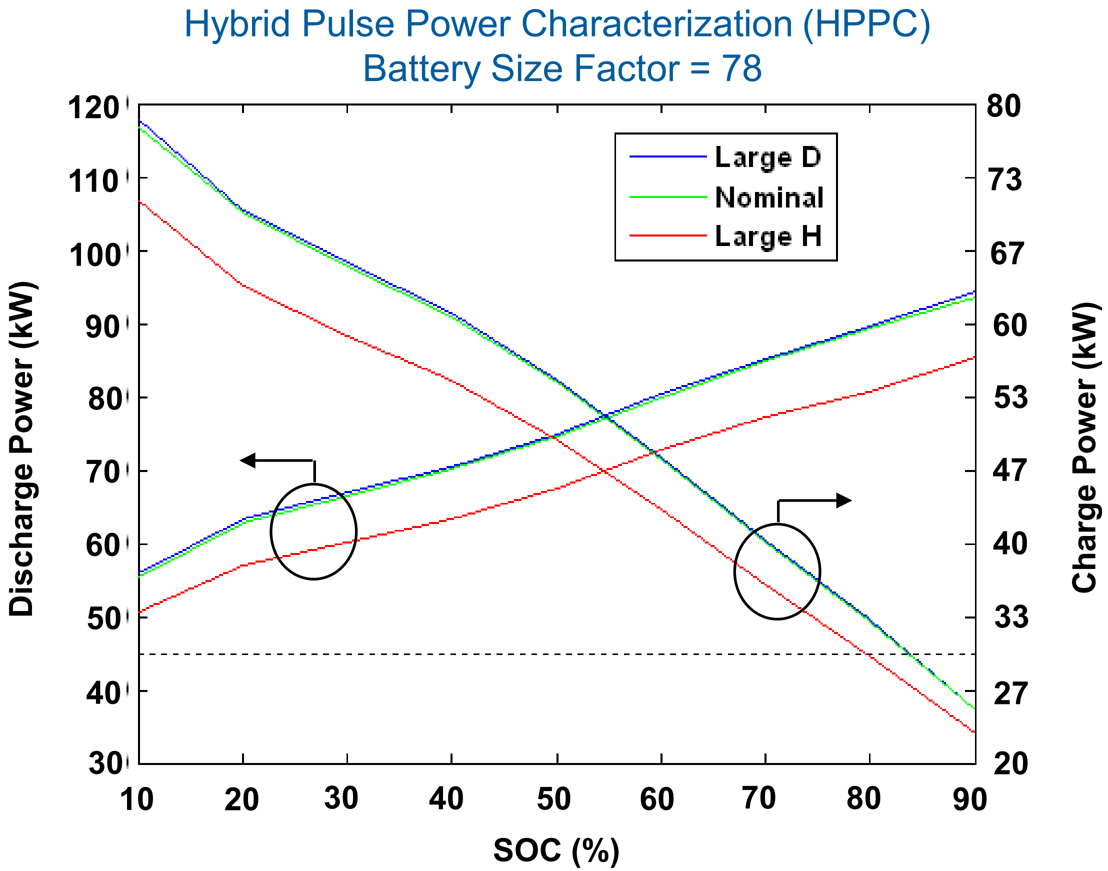


D[mm]: 50
H[mm]: 107

Large D



D[mm]: 115
H[mm]: 20

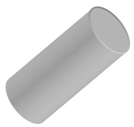


- Large H design has almost 10% less power capability.

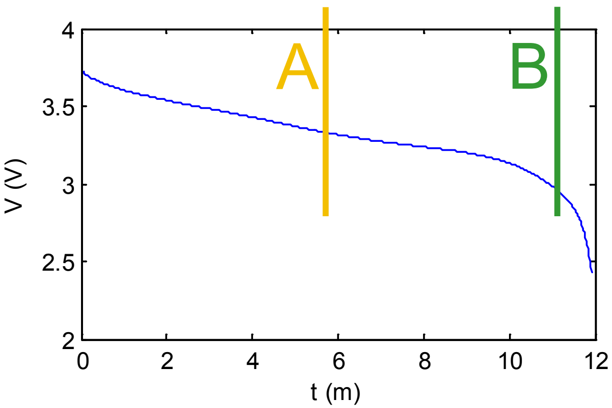
Impacts of "Aspect Ratio" of a Cylindrical Cell

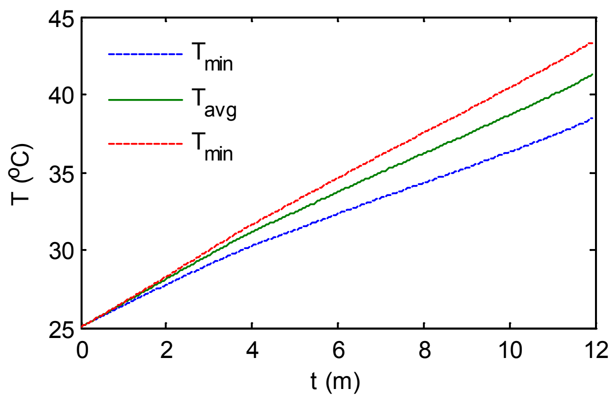
- *Constant Discharge Simulation*
- *Standard Vehicle Driving Profile Simulation*

5C Discharge



– Nominal Cell





Temperature, $T-T_{avg}$

+ A

-

B

Reaction Current, $(i-i_{avg})/i_{avg}$ [%]

A

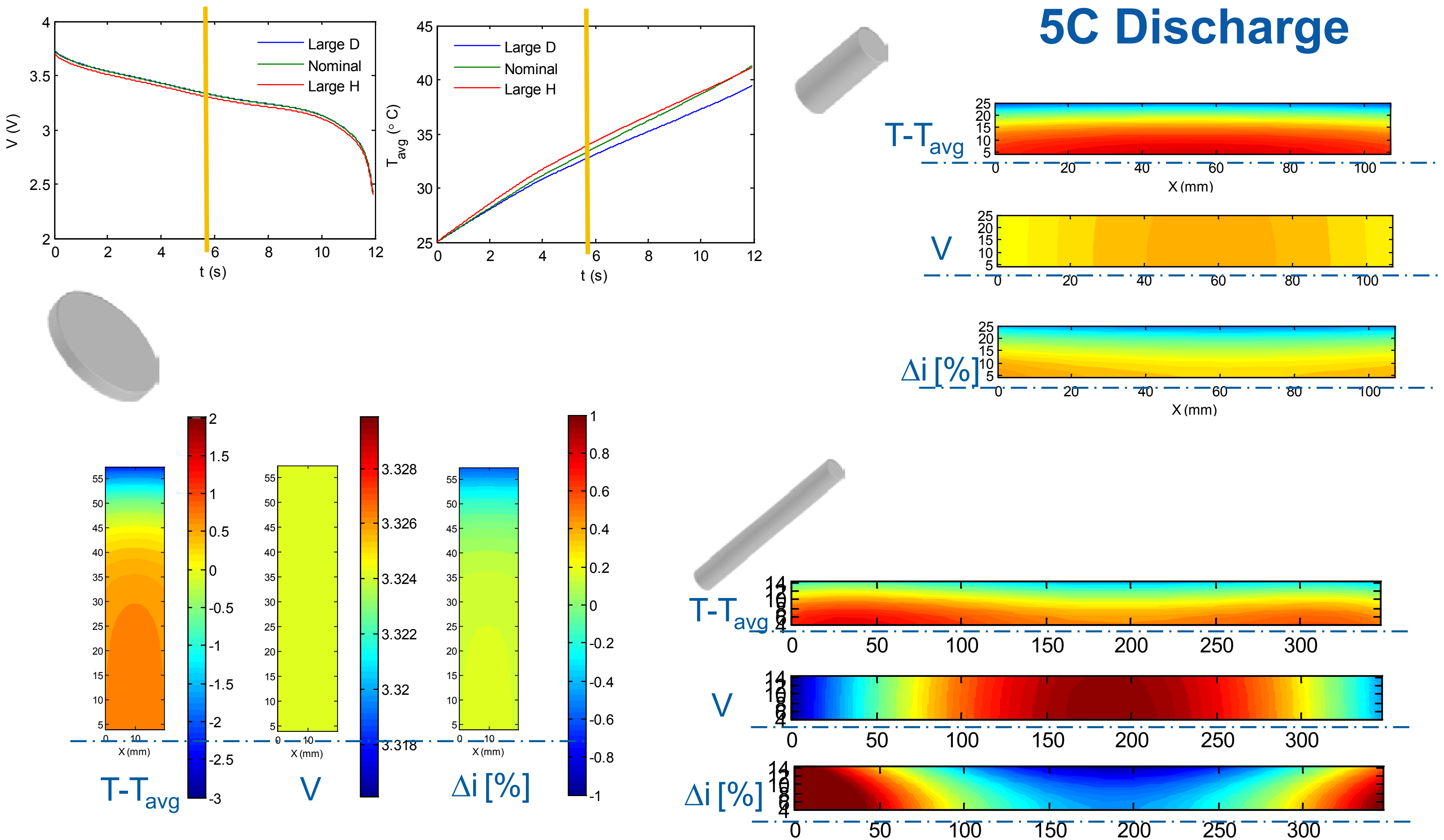
B

Working Potential

A

Snapshot Comparison for H/D ratio

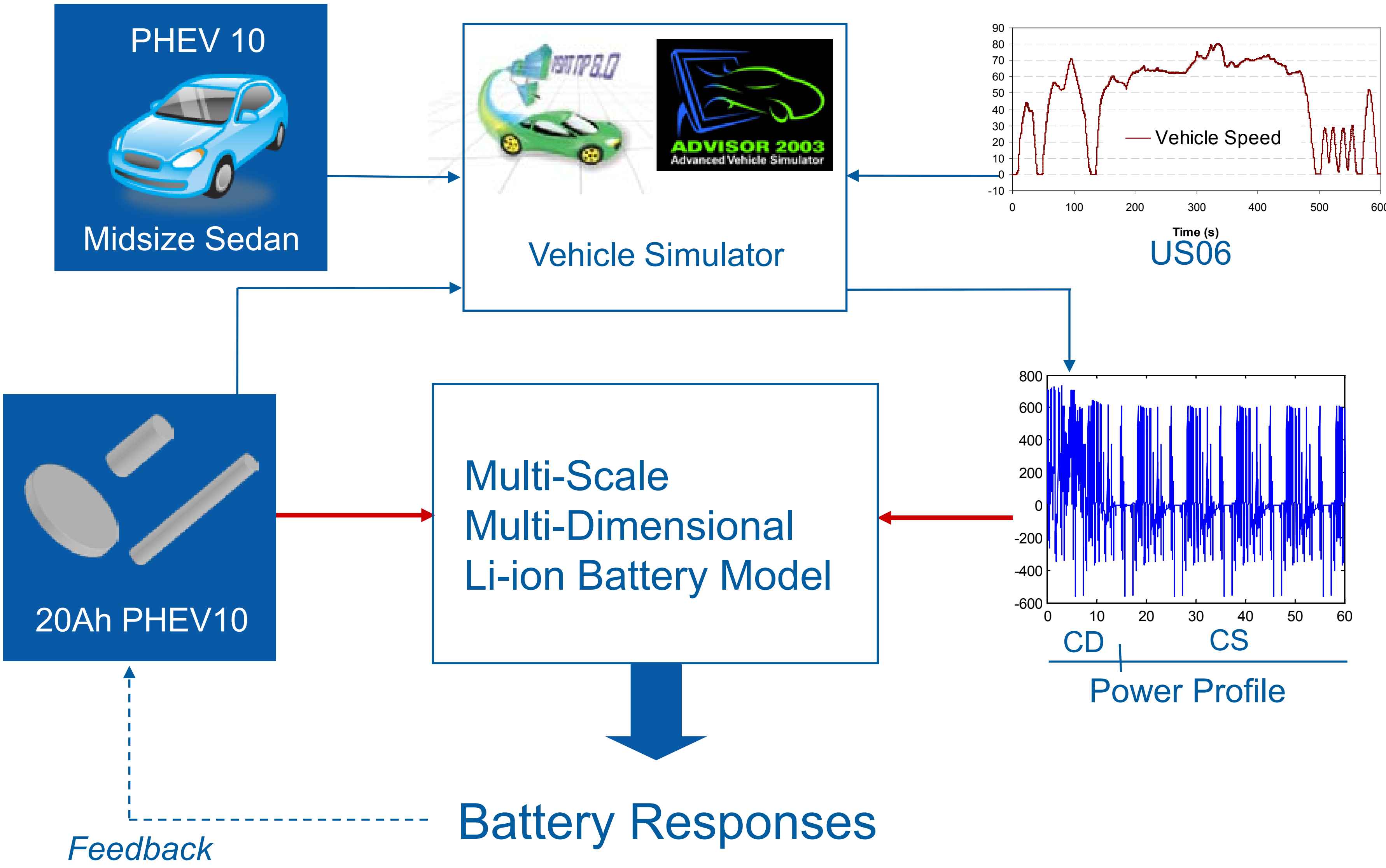
5C Discharge



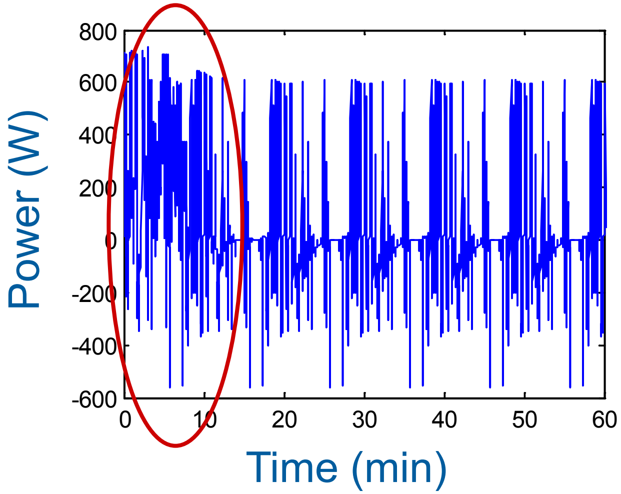
Impacts of “Aspect Ratio” of a Cylindrical Cell

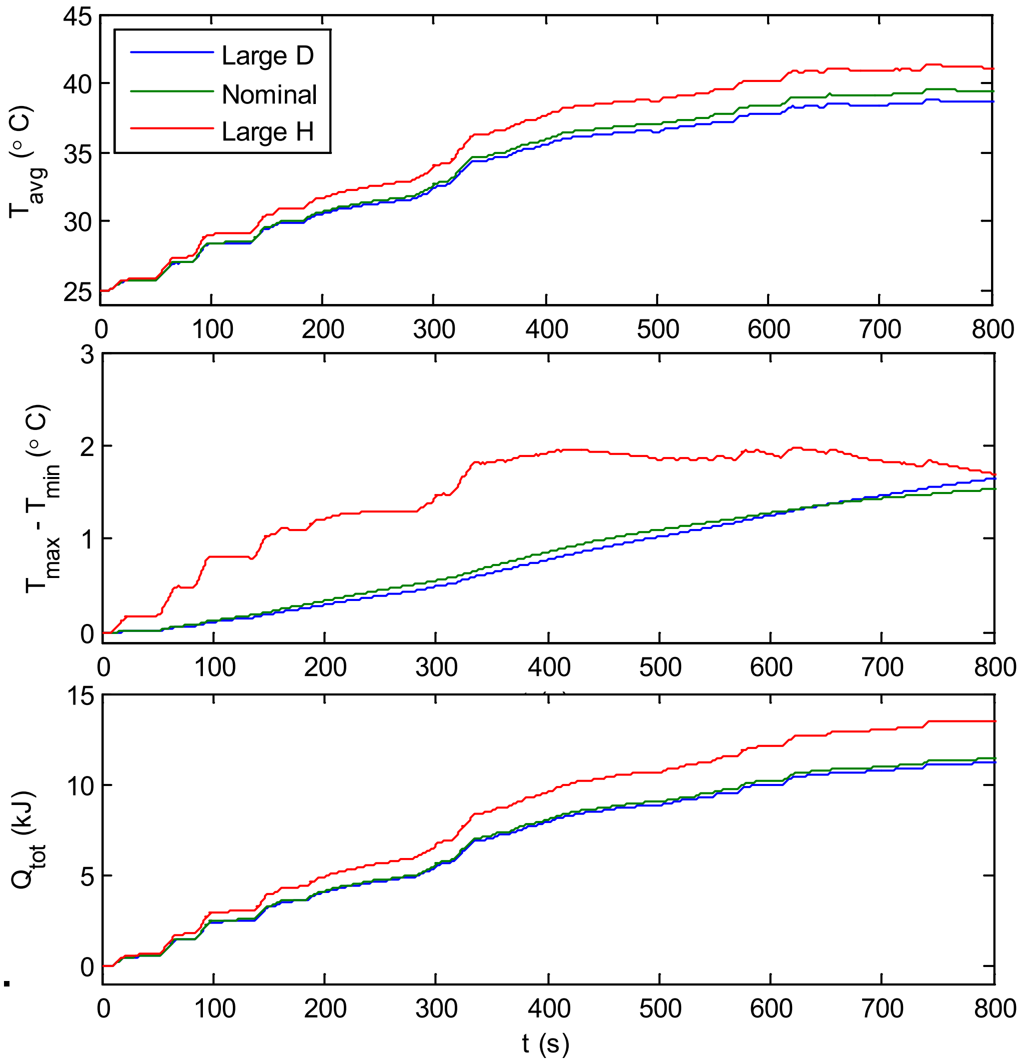
- *Constant Discharge Simulation*
- *Standard Vehicle Driving Profile Simulation*

Approach Virtual Design Evaluation



US06 Charge-Depleting Cycle



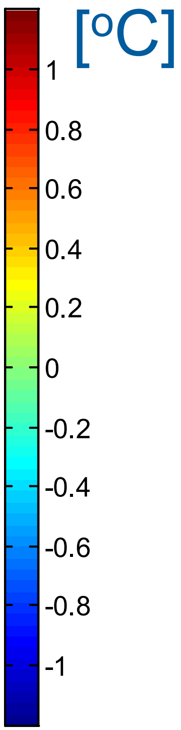


Large H cell has greatest temperature rise because long electronic current paths result in high foil heating.

Large H cell has greatest internal temperature imbalance.

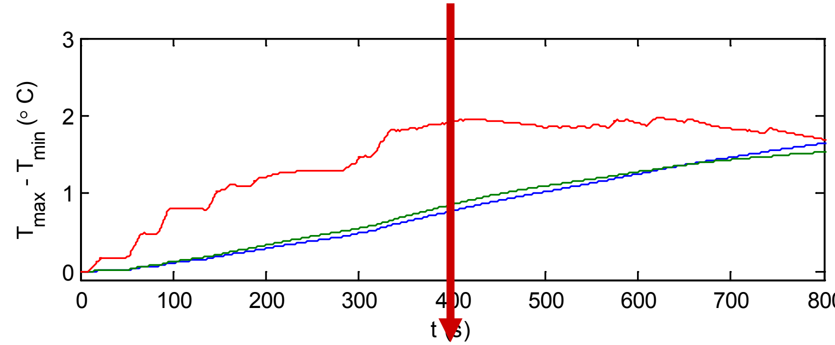
Instant Temperature Imbalance

Temperature Imbalance

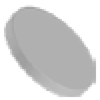


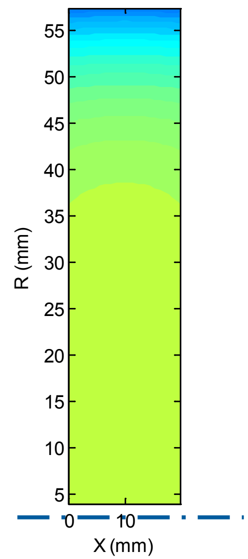
US06 CD cycle

$T - T_{avg}$

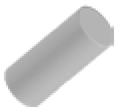


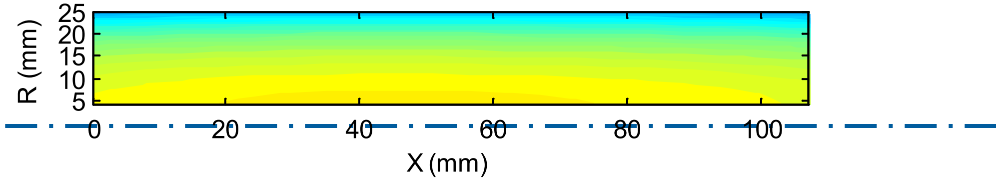
Large Dia. Cell
T_{avg} = 35.5°C



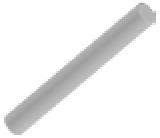


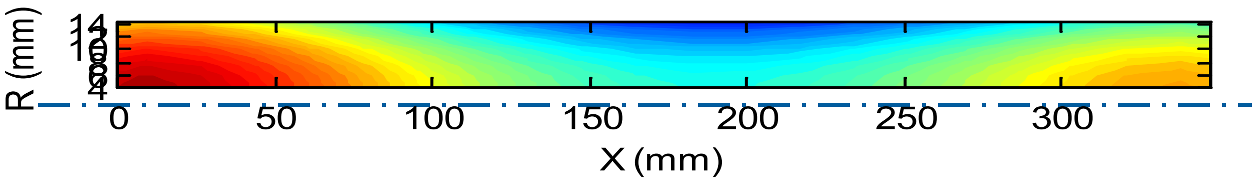
Nominal Cell
T_{avg} = 35.9°C





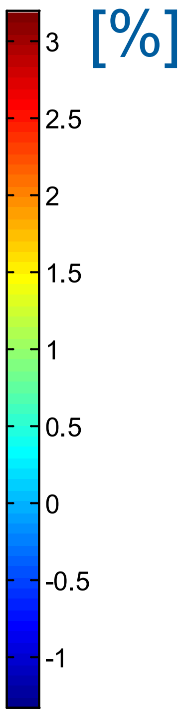
Large Height Cell
T_{avg} = 37.6°C





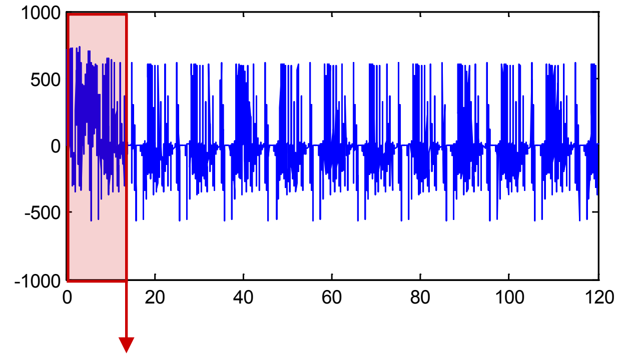
Material Usage Imbalance

Amp-hour Throughput Imbalance

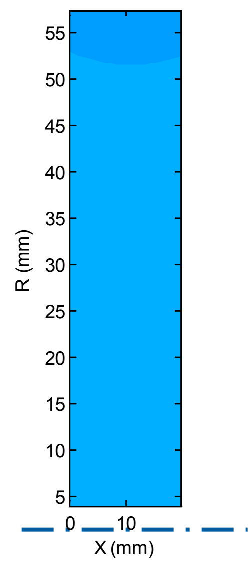


US06 CD cycle

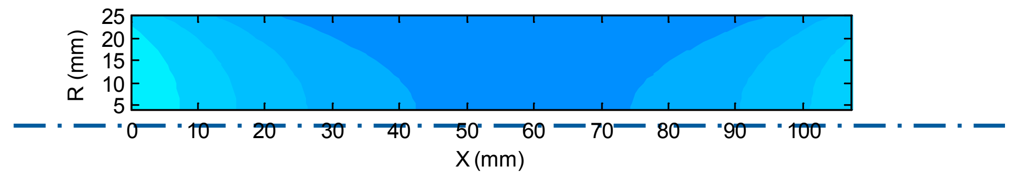
$(Ah/m^2 - Ah/m^2_{avg})/Ah/m^2_{avg}$



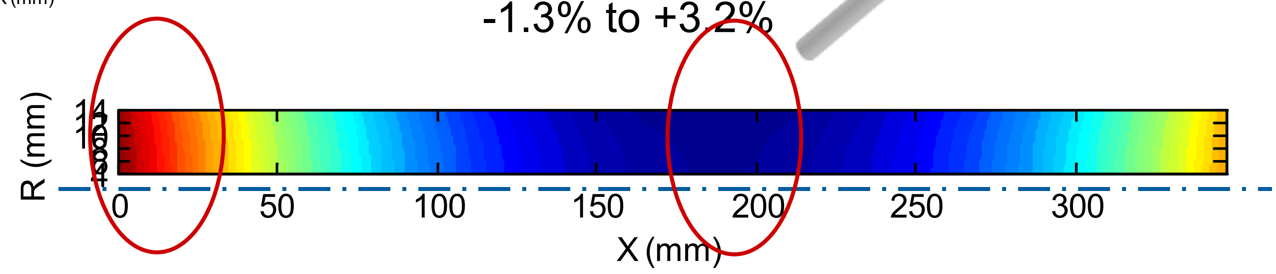
Large Dia. Cell
-0.1% to +0.03%



Nominal Cell
-0.20% to +0.33%



Large Height Cell
-1.3% to +3.2%



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 developed as a tool for investigating interactions between micro-scale electrochemical processes and macro-scale transports using a multi-scale modeling scheme.
- The developed model is used to provide a better understanding and help answer engineering questions about improving *the design*, *operational strategy*, *management*, and *safety* of cells.

- Engineering questions to be addressed in *future work* include …

What is the optimum form-factor and size of a cell?
Where are good locations for tabs or current collectors?
How different are measured parameters from their nonmeasurable internal values?
Where is the effective place for cooling? What should the heat-rejection rate be?
How does the design of thermal and electrical paths impact under-current-related safety events, such as internal/external shorts and overcharge?

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