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NATIONAL RENEWABLE ENERGY LABORATORY

EVS 25
Sustainable Mobility Revolution
November 5-9, 2010 Shenzhen, China

Accelerating Design of Batteries Using Computer-Aided Engineering Tools

Ahmad Pesaran
Gi-Heon Kim
Kandler Smith

25th Electric Vehicle Symposium
Shenzhen, China
November 5-9, 2010

NREL/PR-5400-50354

This work is funded by U.S. Department of Energy, Vehicle Technologies, Energy Storage R&D (Dave Howell)

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.

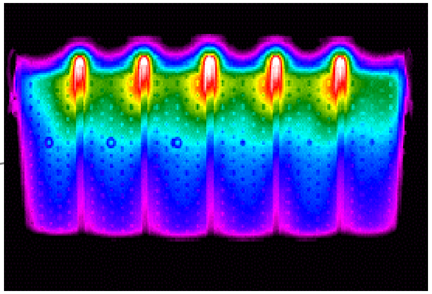
Outline

- Motivation for Battery Computer-Aided Engineering (CAE)
- Multi-Physics Modeling at Various Scales
- NREL Modeling Approach (MSMD)
- Results
  - Impact of Cell Tab Locations
  - Impact of Cell Aspect Ratio
- Conclusions

Motivation for Battery Design Tools

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

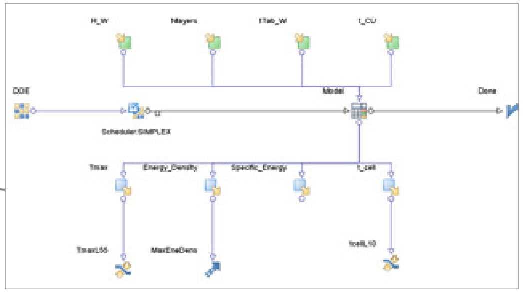
- Large cells/batteries suffer from heat, current, and stress issues not present in small configurations



Thermal Image of Gen I Toyota Prius Module

CAE processes offer a methodology to shorten design cycle and optimize batteries for thermal uniformity, safety, long life, and low cost

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



Process Integration, Design & Optimization (PIDO) Software

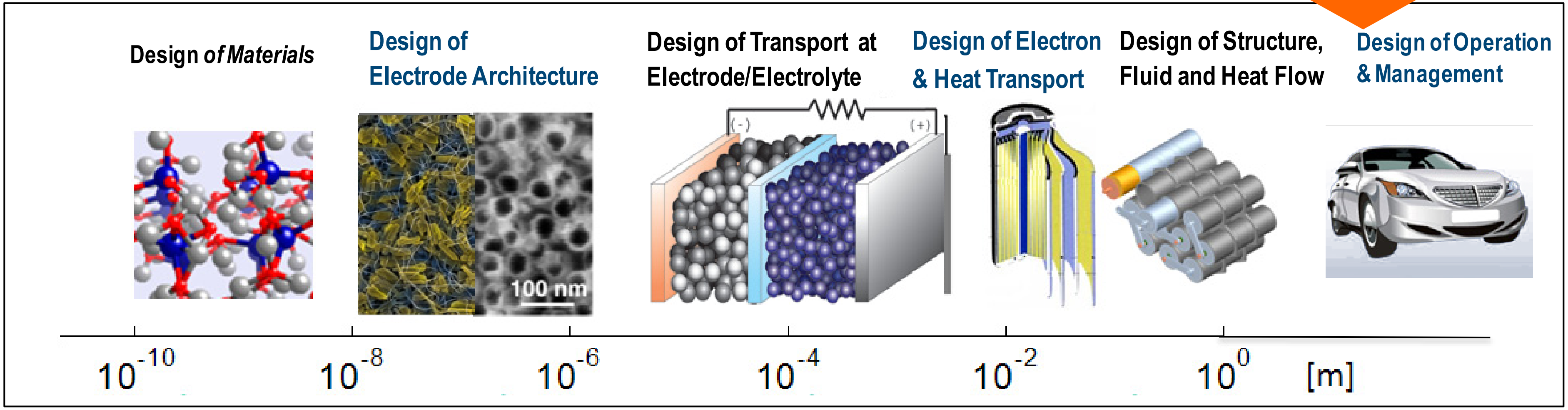
Requirements for large battery CAE:

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

Multi-Scale Physics in Li-Ion Battery

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

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

Virtual Integrated Design
Battery Pack and Vehicle Simulations

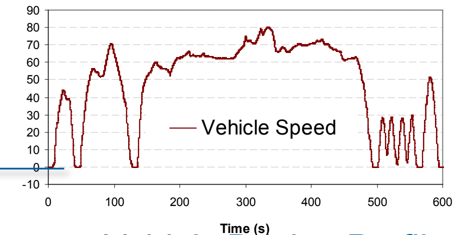
Integrated design approach using a vehicle simulation tool with a battery pack simulation tool that has details of cell-level model embedded in it would be a powerful technique to design batteries

Virtual

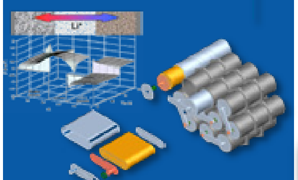
Vehicle Design

Embedded Battery Model

Vehicle Simulator

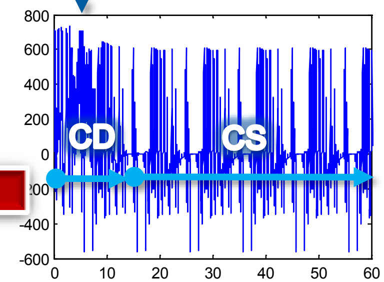


Vehicle Driving Profile



Virtual Battery Design

Multi-Scale
Multi-Dimensional
Li-ion Battery Model



Battery Power Profile

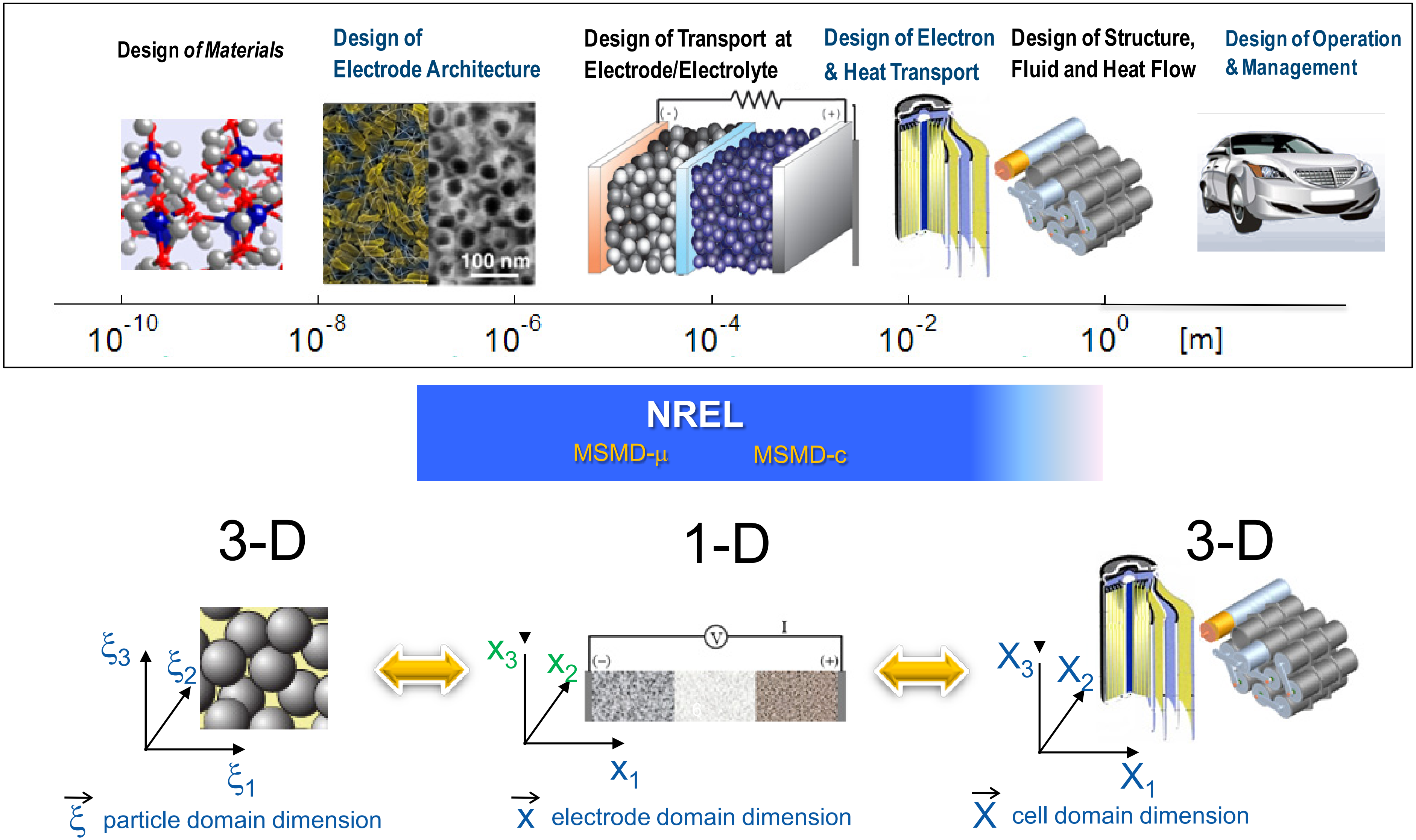
Charge-sustaining
Charge-depleting
Combination charging

Battery Responses

Feedback

NREL's Multi-Scale Multi-Dimensional (MSMD) Model

Efficient representation of 3-D electrochemical/thermal physics

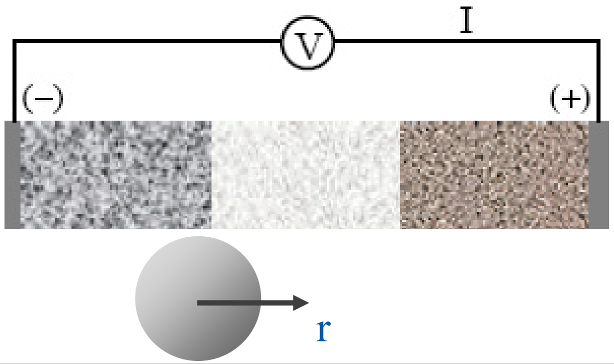


Electrode-Scale Performance Model in the NREL MSMD Model

Charge Transfer Kinetics at Reaction Sites

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

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



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

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

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

- 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

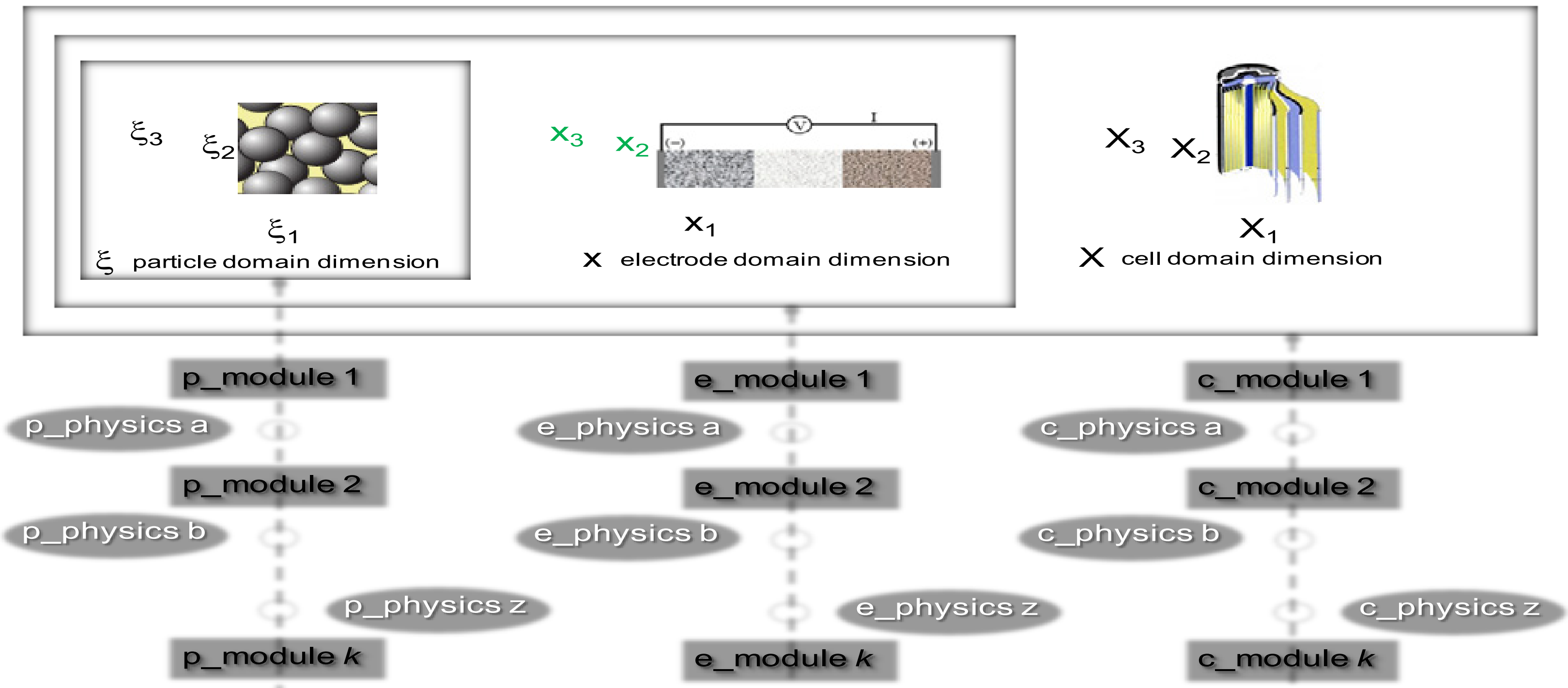
Energy Conservation

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

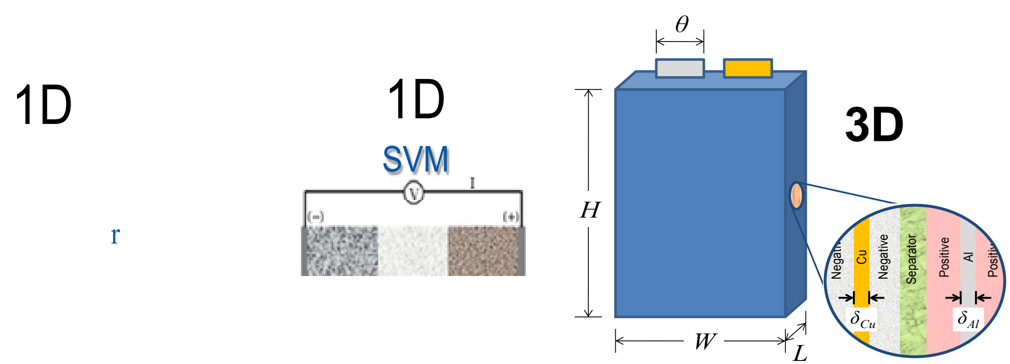
$$q''' = j^{Li}\left(\phi_s - \phi_e - U + T\frac{\partial U}{\partial T}\right) + \sigma^{eff} \nabla \phi_s \cdot \nabla \phi_s + \kappa^{eff} \nabla \phi_e \cdot \nabla \phi_e + \kappa_D^{eff} \nabla \ln c_e \cdot \nabla \phi_e$$

Modularized Hierarchy of Model Structure in NREL's MSMD Approach

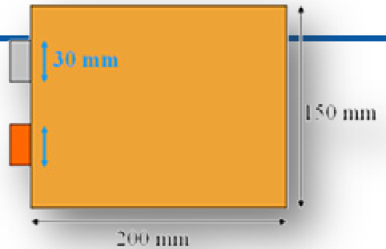
- General Model



- For This Study

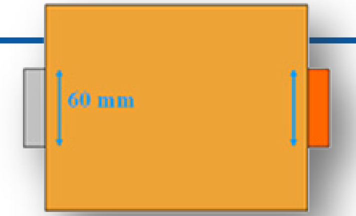


Results: Impact of Tab Location—Importance of Multi-Physics Interaction



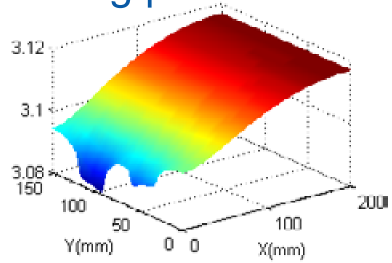
Comparison of two 40-Ah flat-cell designs

2 min 5C discharge

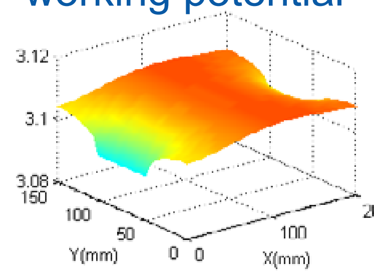


- *Larger over-potential promotes faster discharge reaction*
- *Converging current causes higher potential drop along the collectors*

working potential

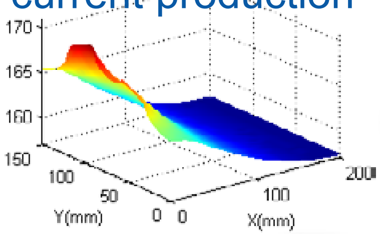


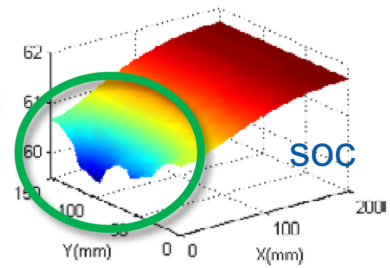
working potential

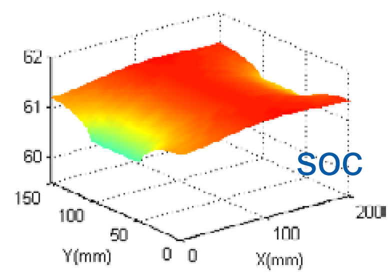


This cell is cycled more uniformly, can therefore use less active material ($) and is expected to have longer life.

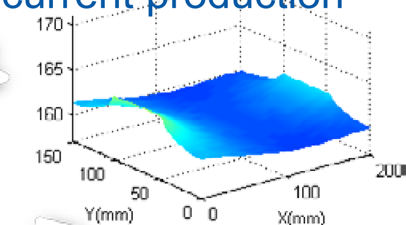
electrochemical current production





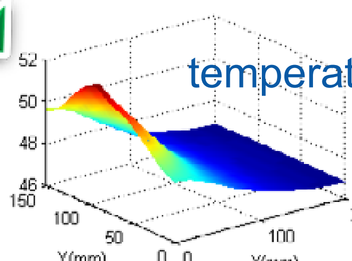


electrochemical current production

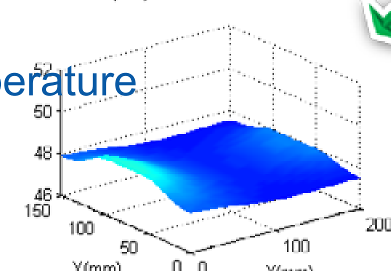


- *High temperature promotes faster electrochemical reaction*
- *Higher localized reaction causes more heat generation*

temperature

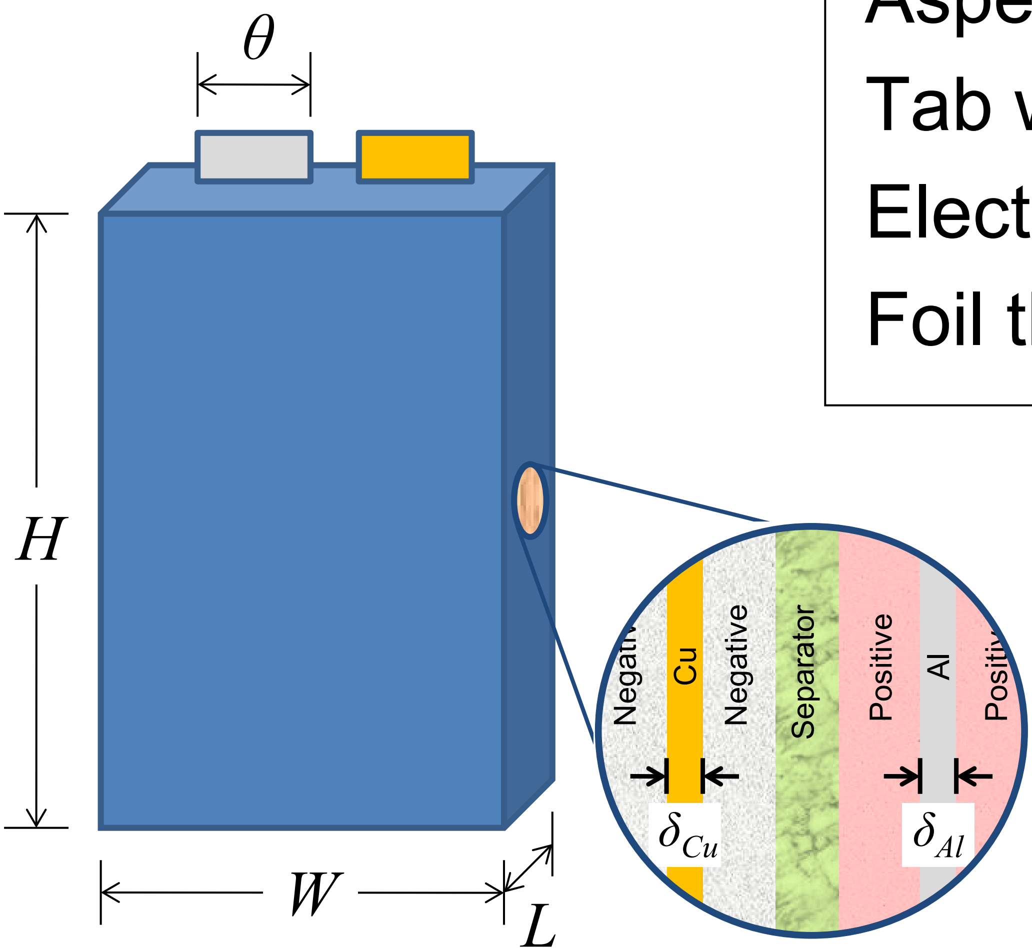


temperature



nickel-cobalt-aluminum (NCA) cathode and graphite anode

Macroscopic Parameters for Design



Aspect ratio, H/W

Tab width, θ/W

Electrode layers, N

Foil thickness, δ_{Cu}

Other design parameters fixed:

- δ_{Al} = 1.6 x δ_{Cu}
- 20-Ah capacity
- Electrode loadings
- Electrode thicknesses

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

Design Impact of Alternative Aspect Ratio

1. Nominal Design

- 140 x 100 x 15 mm^3
- Tabs on the same side
- 20 Ah
- Nominal area and thickness

2. Small Capacity

- 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

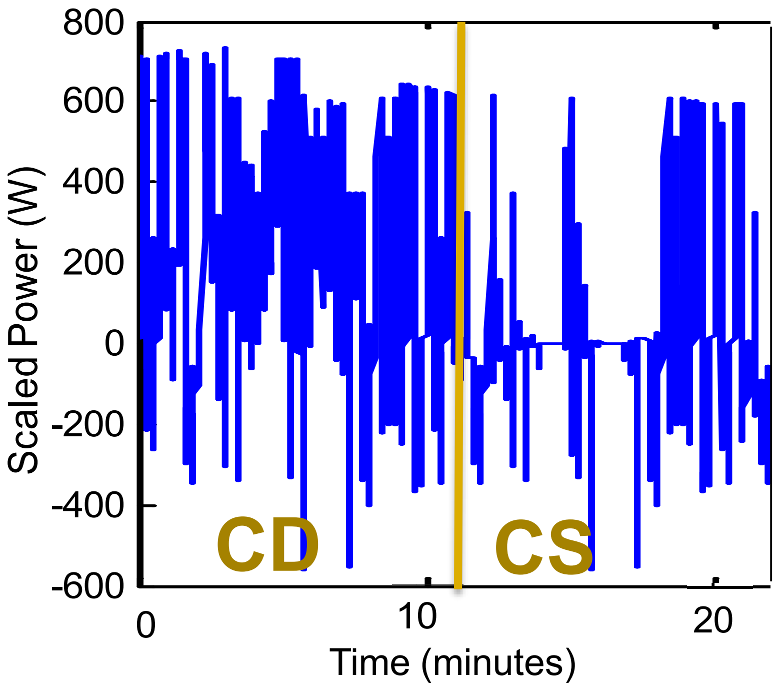
3. Thinner & Wider

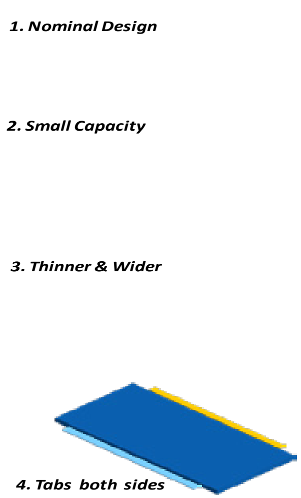
- 200 x 140 x 7.5 mm^3
- Same tabs
- 20 Ah
- 2x electrode area/stack layer
- 1/2 thickness
- ~ 2x surface area

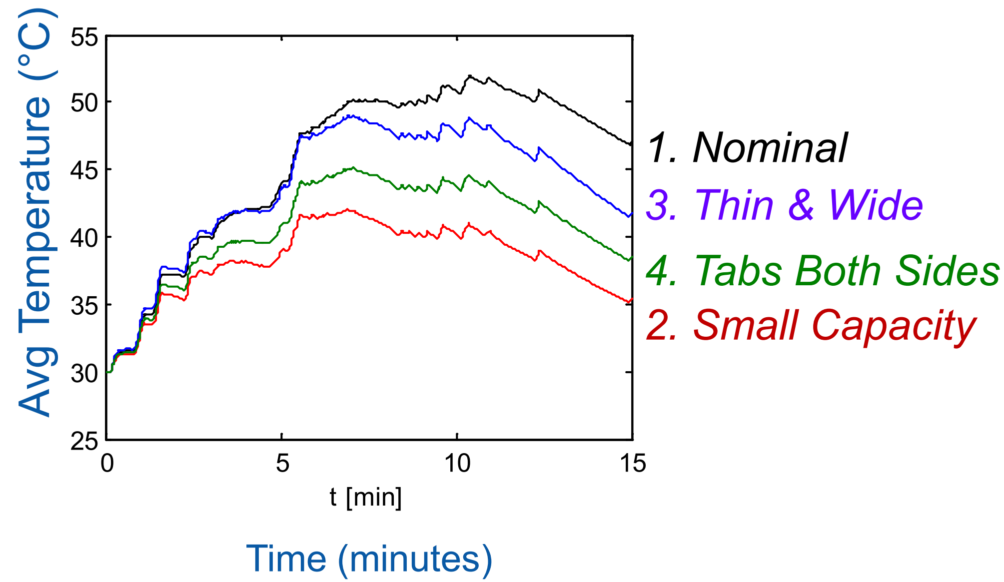
4. Tabs both sides

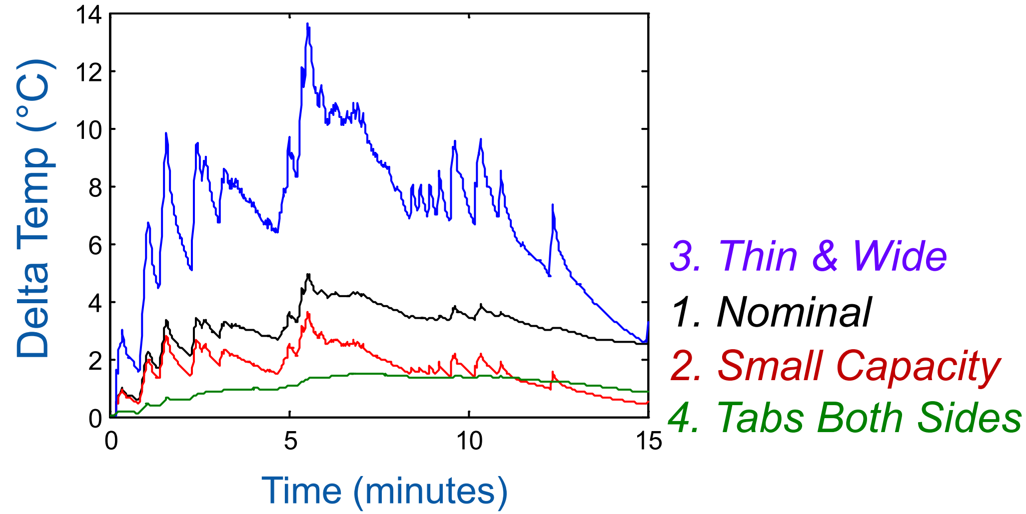
- 250 x 120 x 7 mm^3
- Wide-counter tab design
- 20 Ah
- ~2x electrode area/stack layer
- ~1/2 thickness
- ~2x surface area

Results: Impact of Aspect Ratio



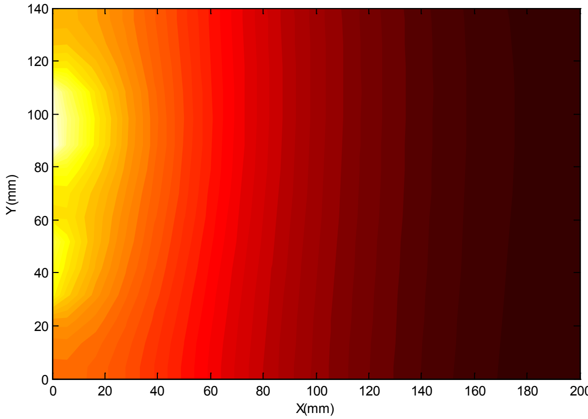




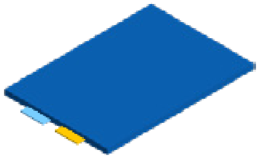


Imbalance Between 20-Ah Designs

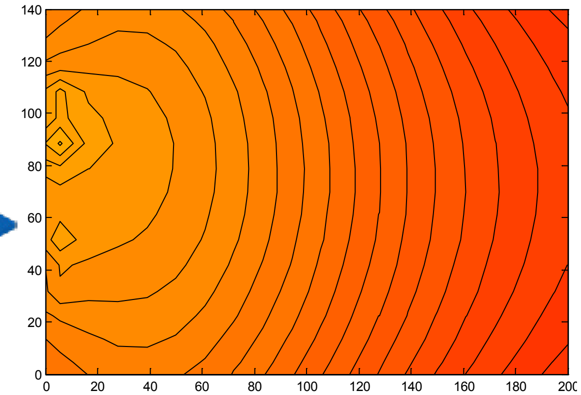
Current Density (Ah/m²)

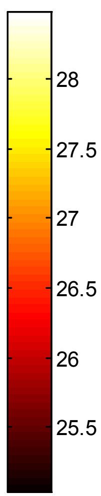


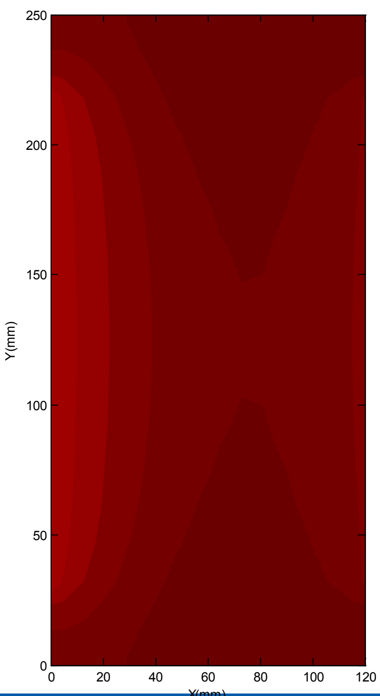
Thin and wide



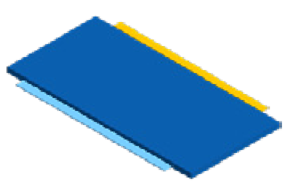
Temperature (°C)

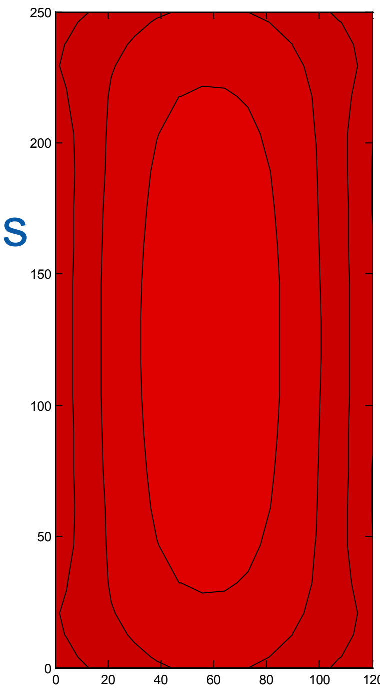


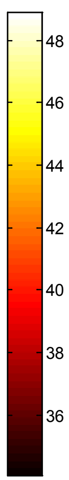




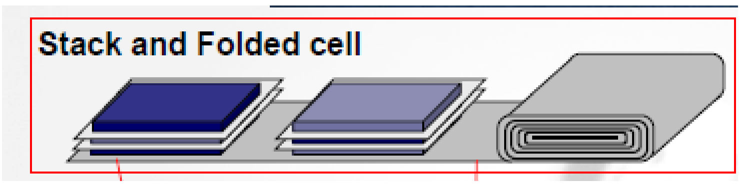
Tabs on both sides

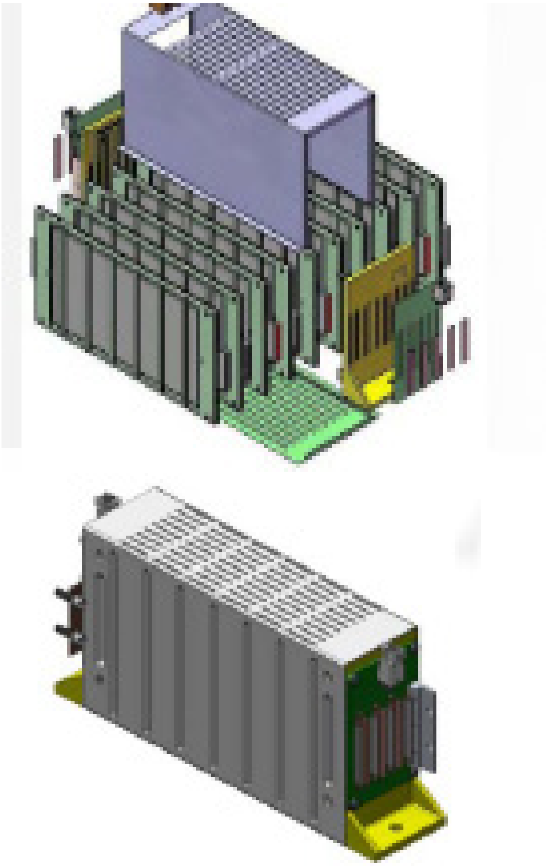


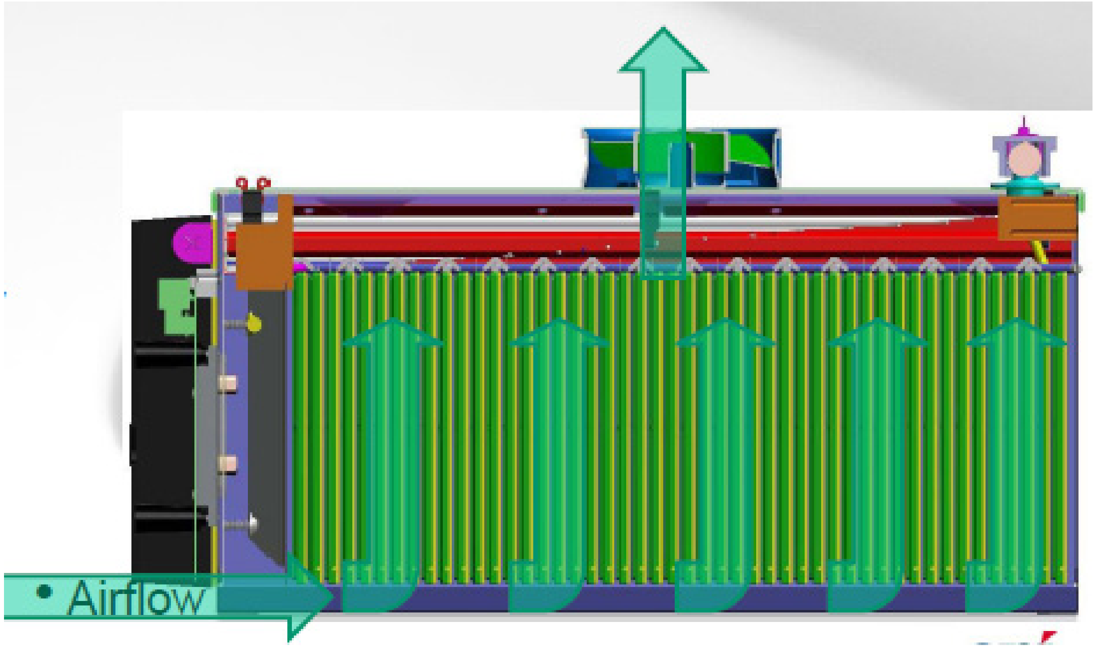




Cell to Pack Modeling Essential for Proper Thermal and Electrical Operations





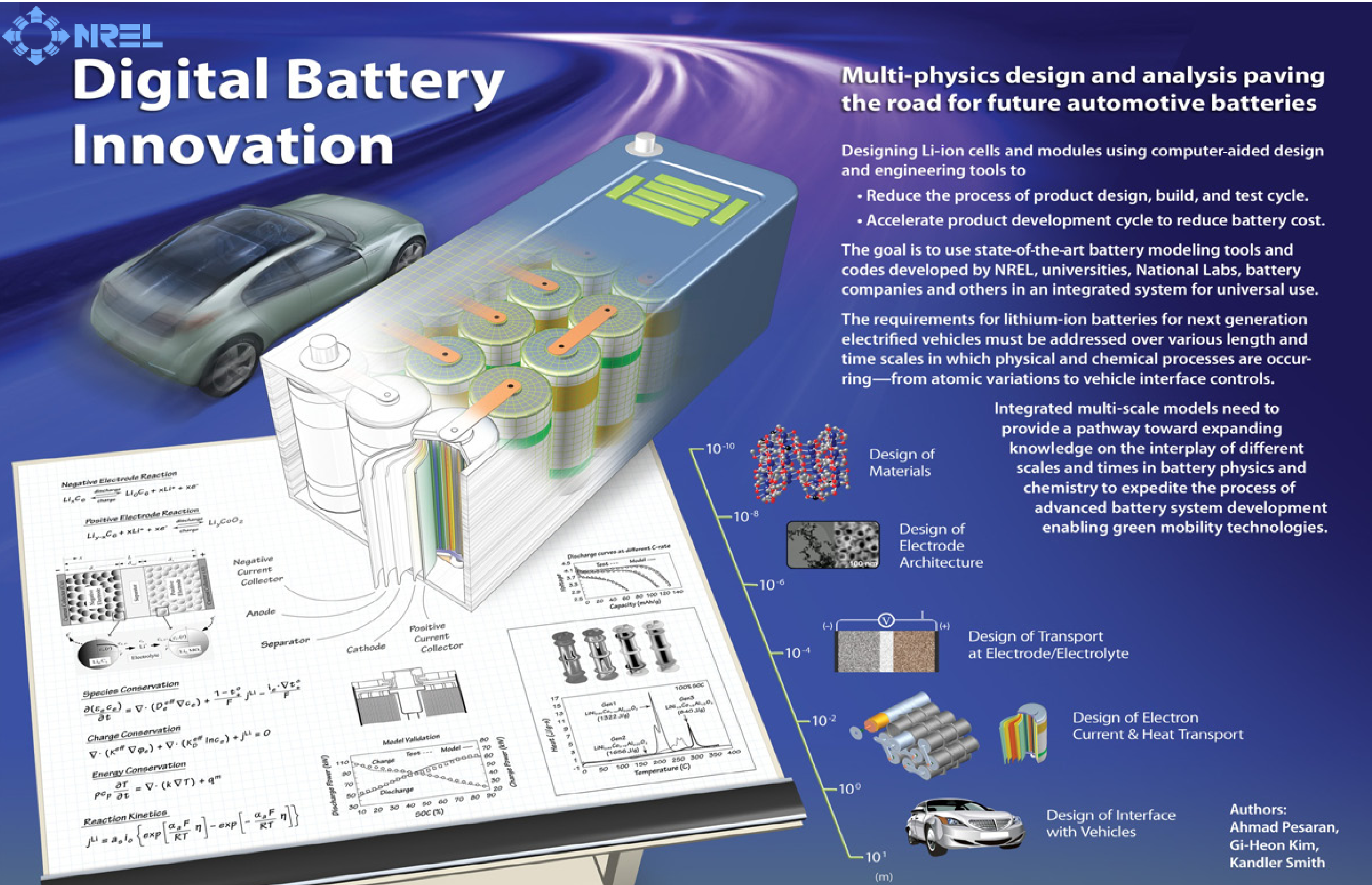


Summary

- Non-uniform battery physics, which is more probable in large-format cells, can cause unexpected performance and life degradations in lithium-ion batteries.
- Computer-aided engineering could investigate various design options quickly before fabrication and testing.
- A Multi-Scale Multi-Dimensional model was used for evaluating large-format prismatic automotive cell designs by integrating micro-scale electrochemical processes and macro-scale transports.
- A 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 the future using 3-D modeling 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?*

Thank You!


NREL
Digital Battery Innovation
Multi-physics design and analysis paving the road for future automotive batteries
Designing Li-ion cells and modules using computer-aided design and engineering tools to
• Reduce the process of product design, build, and test cycle.
• Accelerate product development cycle to reduce battery cost.
The goal is to use state-of-the-art battery modeling tools and codes developed by NREL, universities, National Labs, battery companies and others in an integrated system for universal use.
The requirements for lithium-ion batteries for next generation electrified vehicles must be addressed over various length and time scales in which physical and chemical processes are occurring—from atomic variations to vehicle interface controls.
Integrated multi-scale models need to provide a pathway toward expanding knowledge on the interplay of different scales and times in battery physics and chemistry to expedite the process of advanced battery system development enabling green mobility technologies.
Design of Materials
Design of Electrode Architecture
Design of Transport at Electrode/Electrolyte
Design of Electron Current & Heat Transport
Design of Interface with Vehicles
Authors: Ahmad Pesaran, Gi-Heon Kim, Kandler Smith
Negative Electrode Reaction
Positive Electrode Reaction
Negative Current Collector
Anode
Separator
Cathode
Positive Current Collector
Species Conservation
Charge Conservation
Energy Conservation
Reaction Kinetics
Model Validation
Discharge curves at different C-rate
Temperature (C)
SOC (%)
Capacity (mAh/g)
(m)