Development of Cell/Pack Level Models for Automotive Li-Ion Batteries with Experimental Validation

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EC Power

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5/15/12

Project ID #
ES120

Overview

Timeline

- Start date: 5/1/2011
- End date: 4/30/2014
- 33% complete

Barriers

- Barriers addressed
  - LiB Performance and Lifetime
  - LiB Efficiency
  - LiB Safety
  - Computer tools for design exploration

Budget

- Total project funding: $3.0M
  - $1.5M (DOE)
  - $1.5M (cost share)
- Funding received in FY11
  - $193.6K

Partners

- Ford
- Johnson Controls
- Penn State
- NREL
- ORNL

Funding provided by **Dave Howell** of the DOE Vehicle Technologies Program .
The activity is managed by **Brian Cunningham** of Vehicle Technologies.
Subcontracted by NREL, **Shriram Santhanagopalan** Technical Monitor

Project Objectives - Relevance

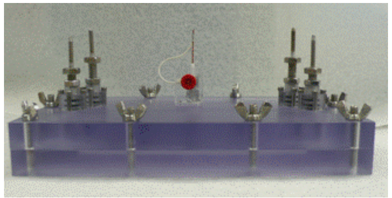
- Develop an electrochemical/thermal (ECT) coupled model for large-format automotive Li-ion batteries (cells and packs)
- Create a fast & robust tool for realistic geometries (wound or stacked electrode designs)
- Develop a comprehensive materials database
- Integrate ECT3D software with CAEBAT Open Arch. Software
- Aide OEMs and cell/pack developers in accelerating the adoption of large-format Li-ion technology required for EV & PHEV
- Develop a virtual environment to reduce the time required for design, build and test of Li-ion batteries
  - Performance
  - Safety
  - Life
  - Efficiency
- Support DOE CAEBAT activity

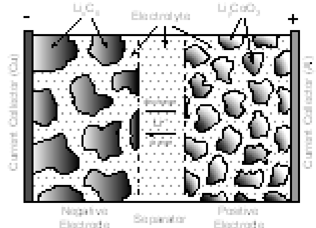
Project Milestones & Activities

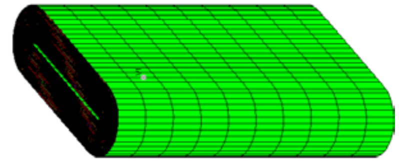
2011/2012 Milestones Completed
M1: Report on initial materials database
M2: Report/manual for baseline ECT3D software delivered to NREL
M3: Baseline ECT3D code delivered to NREL
M4: Updated data for materials database
M5: Report for updated materials database information
M6: Report for updated materials database information
Meetings with ORNL & other CAEBAT members to give input for the Open Architecture Standard
Battery Safety 2011 – Las Vegas (11/2011)
Presentation to USDrive (12/13/11)

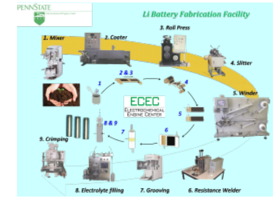
2012 Milestones in Progress
M7: Initial model validation
M8: Report of safety modeling
M9: Updated version of ECT3D to NREL w/pack simulation capabilities
M10: Report for updated materials database information
M11: ECT3D user interfaces complete
M12: Report of detailed model validation for ECT3D

Approach – Supporting CAEBAT Activity









Task 1: Materials Characterization (PSU)

Task 2: Physico-chemical Models (ECP)

Task 3: Advanced Algorithms (ECP)

Task 4: Experimental Validation (PSU, ECP)

EC Power software: ECT3D

Ford, JCI

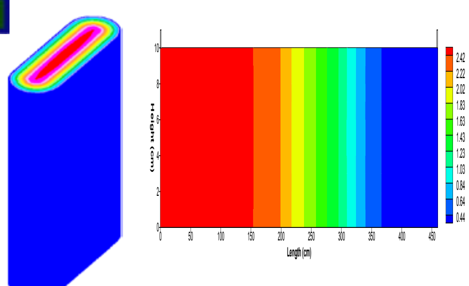
Feedback

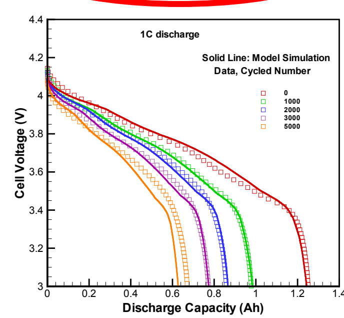
Feedback

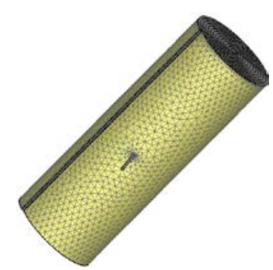
Performance

Cycle Life

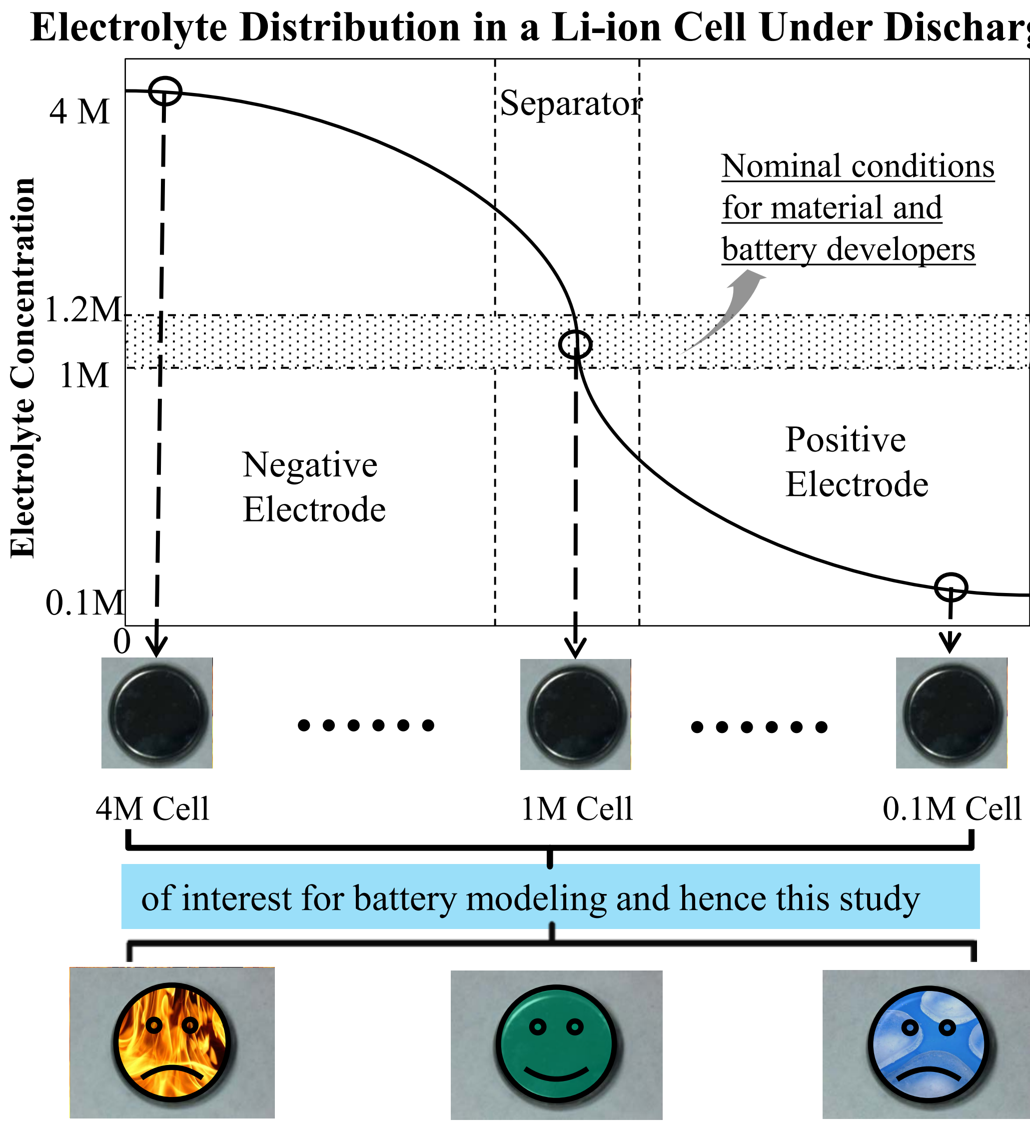
Safety







Approach – Materials Database



Modeling parameters needed at ***low-T, high-T, wide range of chemical compositions*** and similar conditions of interest for ***automotive Li-ion batteries and packs***.

Approach – ECT Model Development

Electrochemical Processes
- electrochemical reactions
- solid state diffusion
- ion transport through electrolyte
- charge transfer

Heat generation rate

$$q = \sum_j a_{sj} \bar{i}_{nj} \left(\bar{\eta}_j + \Pi_j \right) - \sum_k \left[< \mathbf{i}_k > \cdot \nabla < \phi_k >^k \right]$$

Thermal Processes
- conservation of thermal energy

$$\frac{\partial \left(\rho c_p T \right)}{\partial t} = \nabla \cdot \boldsymbol{\lambda} \nabla T + q$$

Temperature-dependent physico-chemical properties

$$\Phi = \Phi_{ref} \exp \left[\frac{E_{act,\Phi}}{R} \left(\frac{1}{T_{ref}} - \frac{1}{T} \right) \right]$$

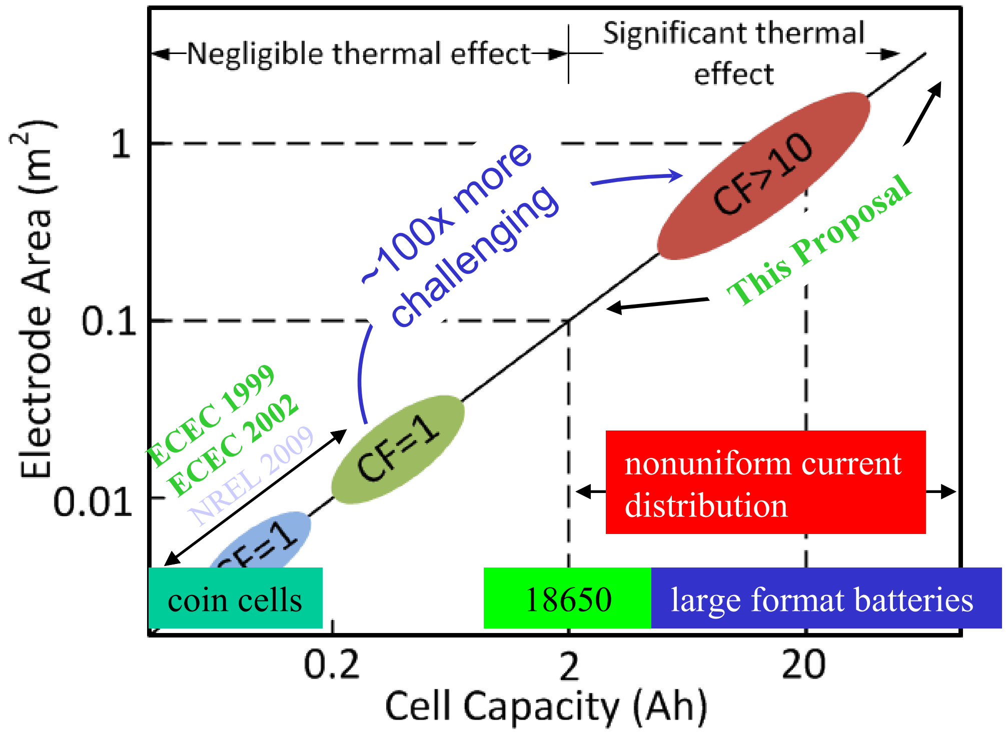
Model predictions
- potential and current curves
- temperature history/distribution
- active material utilization
- current distribution

- Understanding thermal phenomena & thermal control has huge impact on
  - Battery safety
  - Cycle life
  - Battery management system
  - Cost
- Electrochemical-thermal (ECT) coupling required for
  - Internal short circuits
  - Thermal runaway
  - High power, low-T operation
  - Heating from subzero environment

Approach – Computational Challenges

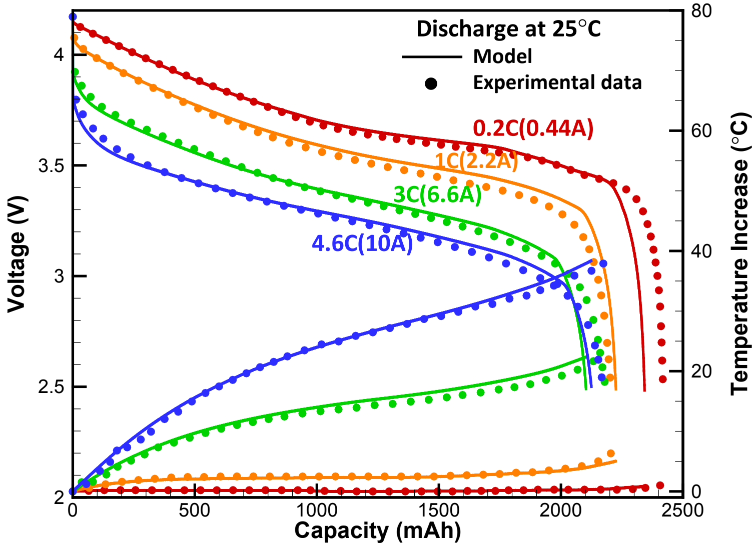
- Develop numerical algorithms to handle:
  1) large electrode size (0.1-1 m^2)
  2) multi-layer wound and stacked geometry
  3) ECT couplings, while still maintaining near **real-time** calculations

$$\text{Compactness Factor (CF)} = \frac{\text{Actual Electrode Area}}{\text{Battery Outer Surface Area}} = \begin{cases} 1 & \text{for coin cells and flat cells} \\ 22.5 \text{ or } 32.5 & \text{for 18650 or 26650 cells} \\ 60\text{-}100 & \text{for pouch cells} \end{cases}$$



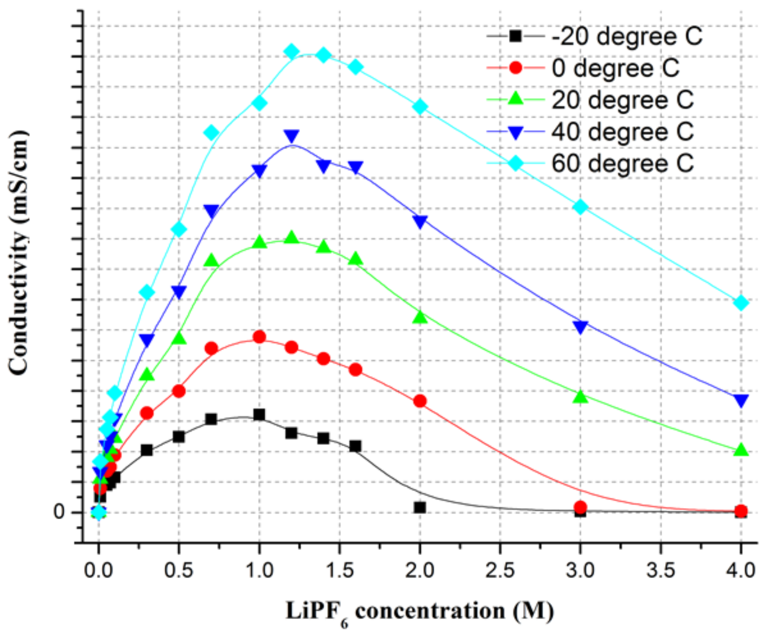
Technical Accomplishments

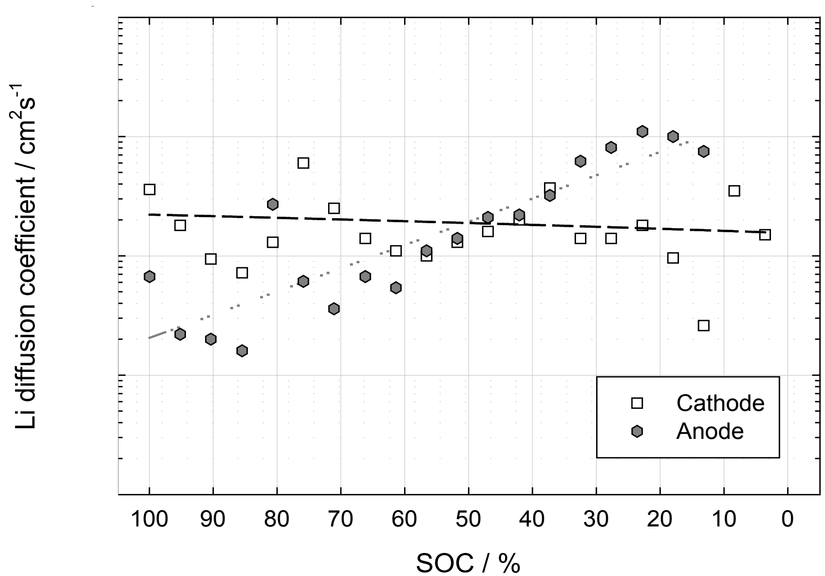
- Development of extensive materials database
- Efficient, electrochemical-thermal coupled large-format cell simulation
  - Performance evaluation and analysis
  - Analysis of active materials utilization
  - Virtual design tool: lower cell cost
- Preliminary validation
- Preliminary safety simulations
  - Full (fast) nail penetration
  - Partial (slow) nail penetration
  - Shorting by metal particle



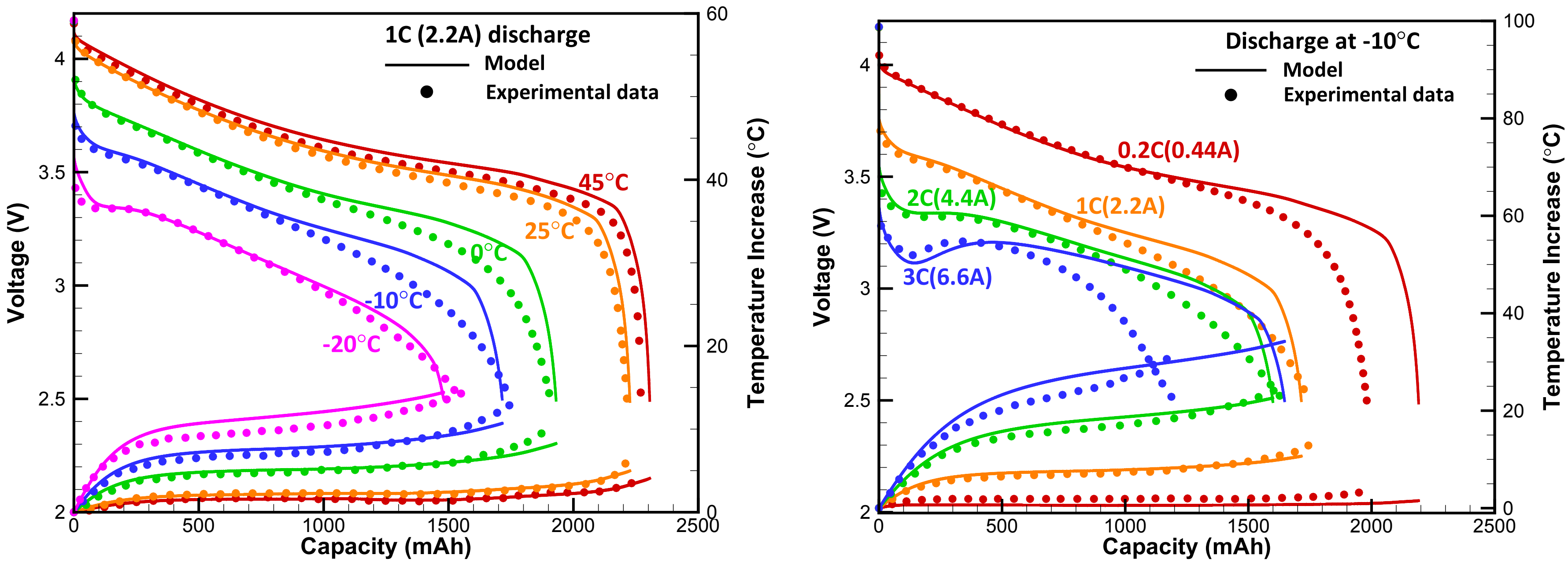
Accomplishments – Material Database

- Material, thermodynamic and kinetic properties for common Li-ion battery materials have been compiled over a wide range of temperature, chemical compositions and SOC.
  - Anode AM: graphite, MCMB, LTO
  - Cathode AM: MNC, LMO, LFP, NCA, LCO
  - Electrolytes: LiPF6 in various solvents





Accomplishments - Validation

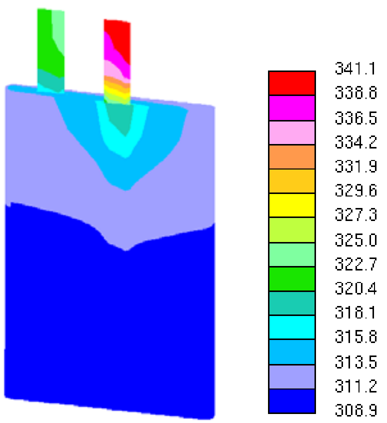


- Initial validation efforts at low-T and high C-rate conditions
- Detailed validation efforts currently ongoing

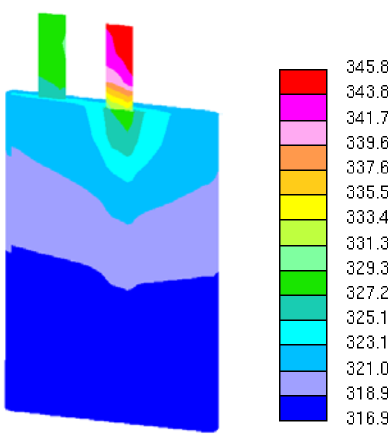
Accomplishments - Performance

3Ah prismatic rolled electrode design – 6C discharge

Temperature (K)

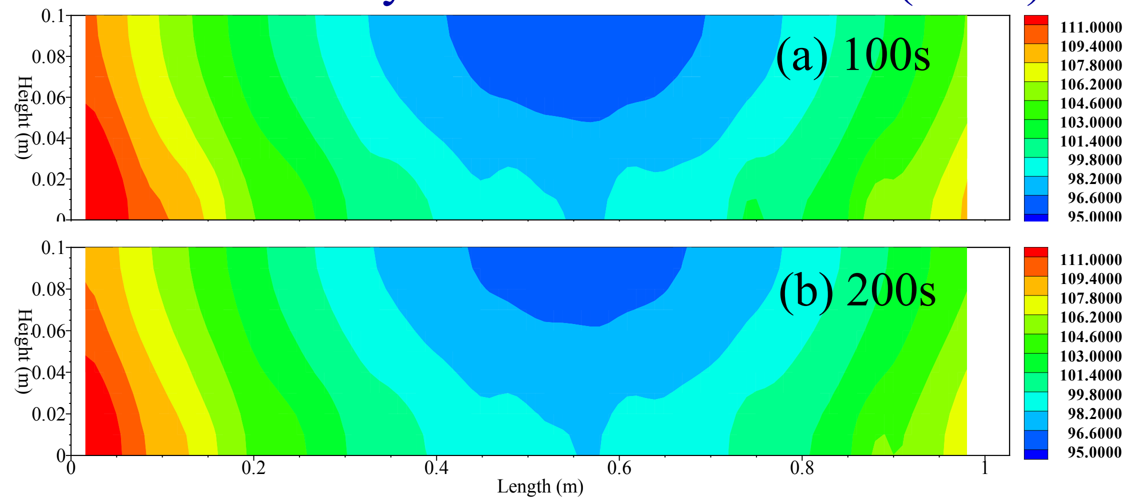


(a) 100s



(b) 200s

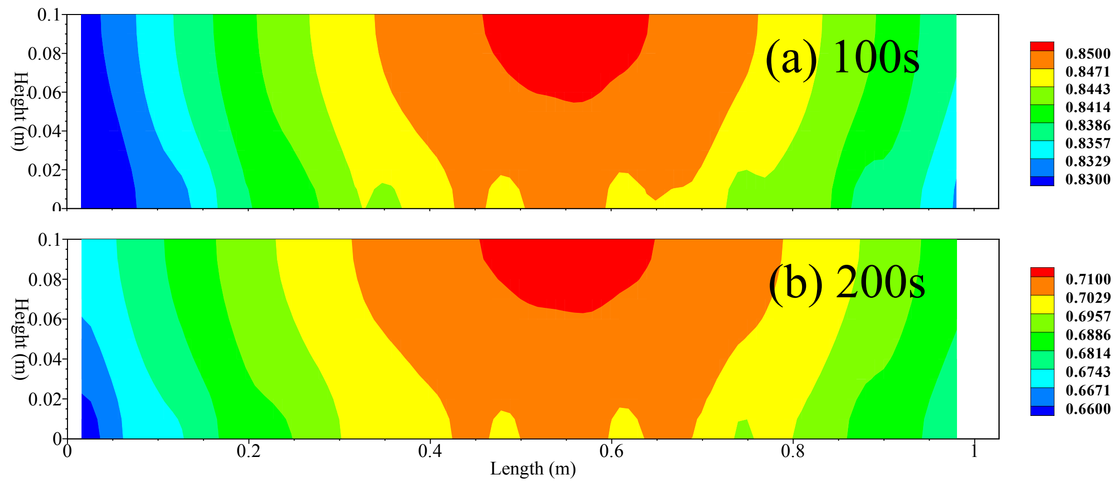
Current Density in Unrolled Electrode (A/m²)



Tab

Tab

SOC in Unrolled Electrode

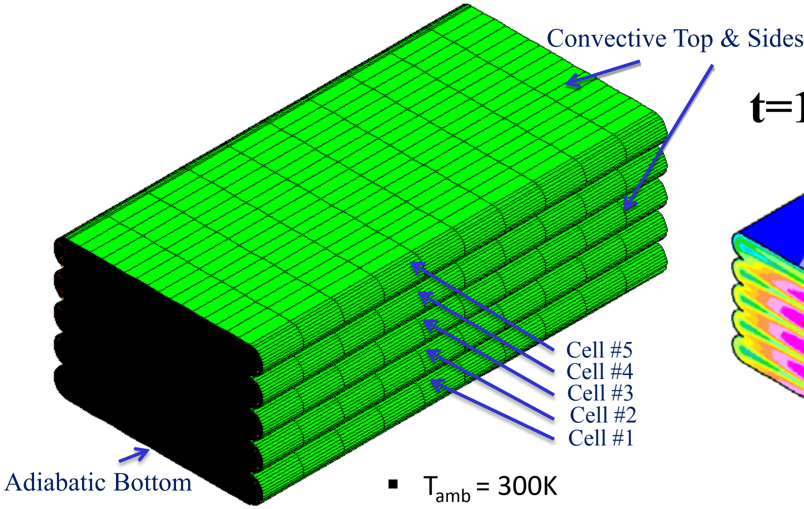


Performance evaluation and local analysis of ***active materials utilization*** over time

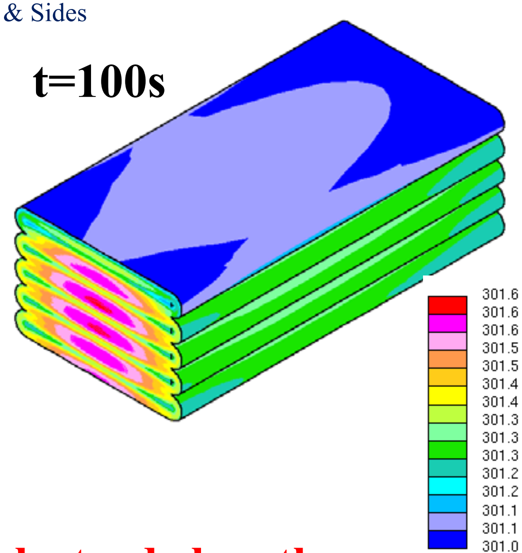
Accomplishments - Performance

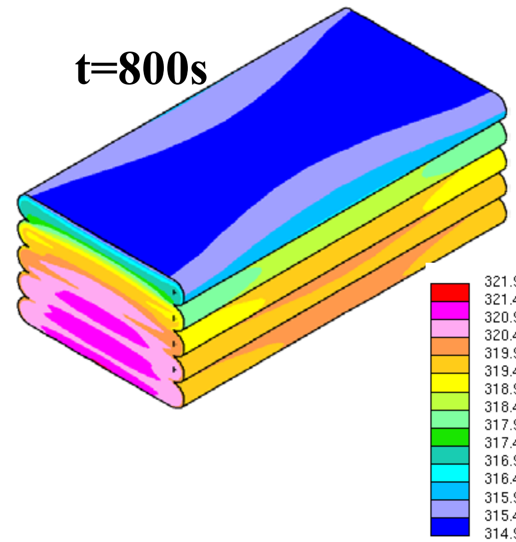
EC POWER

5-Jelly Roll Cell Design (15 Ah)

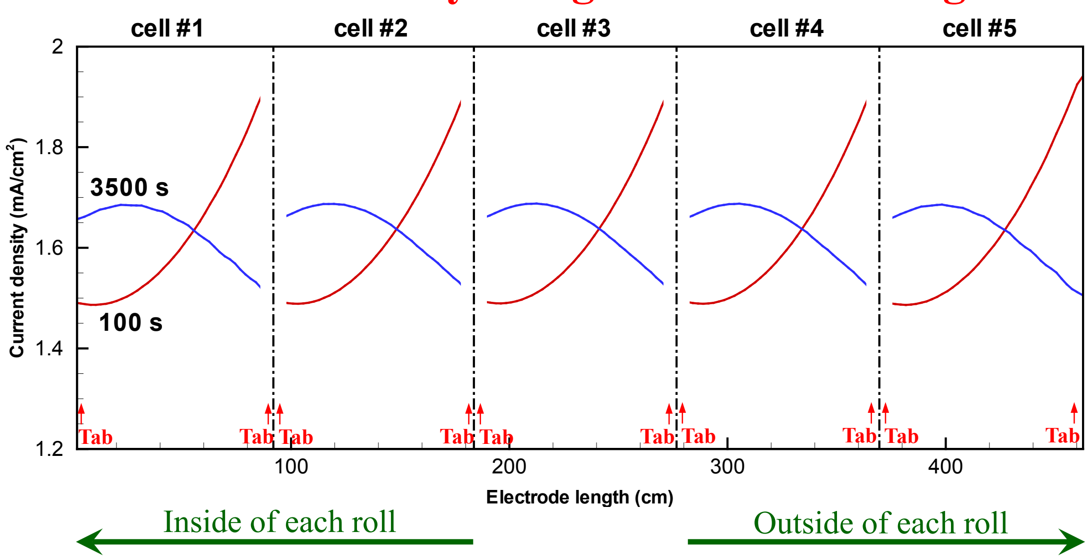


- T_{amb} = 300K
- 1C Discharge





Current density along the electrode length



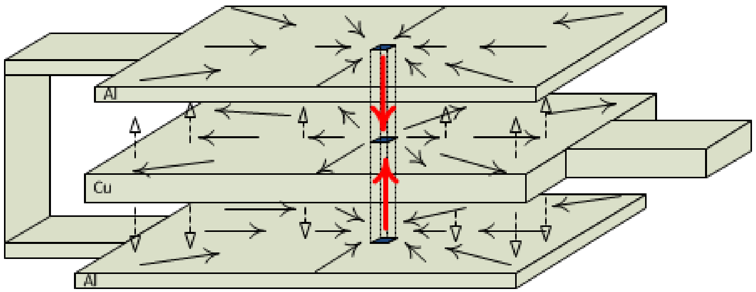
@ t = 100s → Current density profile determined by material and geometric effects

@ t = 3500s → Current density profile determined by material and geometric effects, *local* SOC non-uniformity, and thermal effects

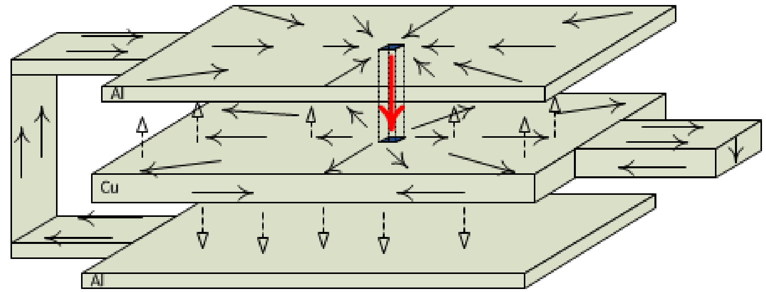
Design optimization for
active materials utilization

Accomplishments - Safety

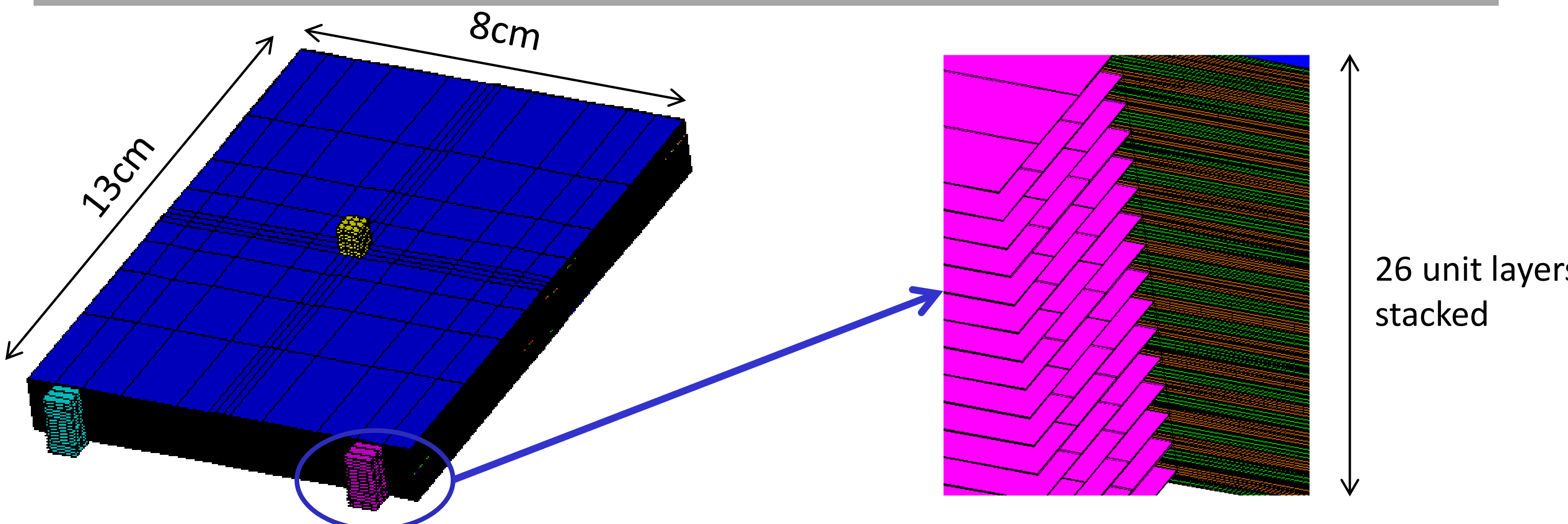
Full nail penetration (Fast)



Partial nail penetration (Slow)



Case Study (10Ah prismatic cell)

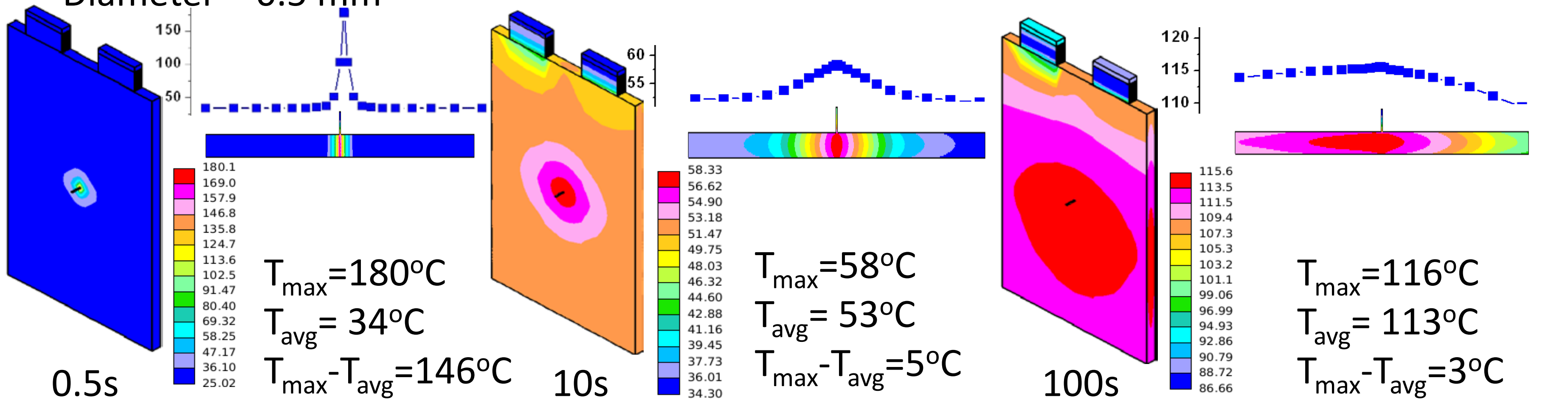


Only ***3-D electrochemical-thermal coupled (ECT) model*** can completely describe the problem

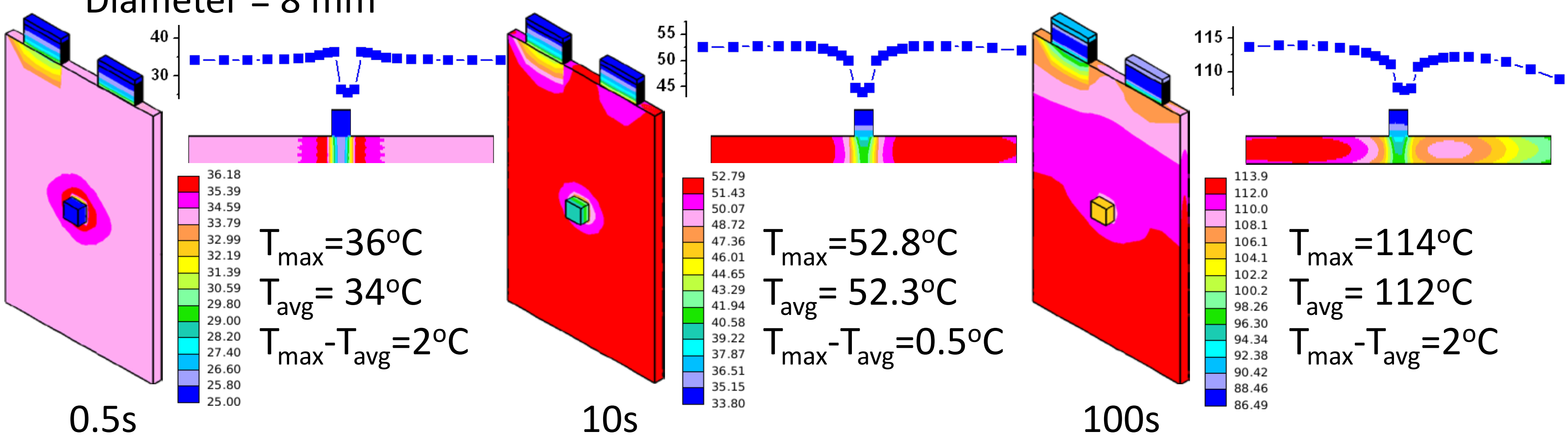
Accomplishments - Safety

Full Penetration

Diameter = 0.5 mm



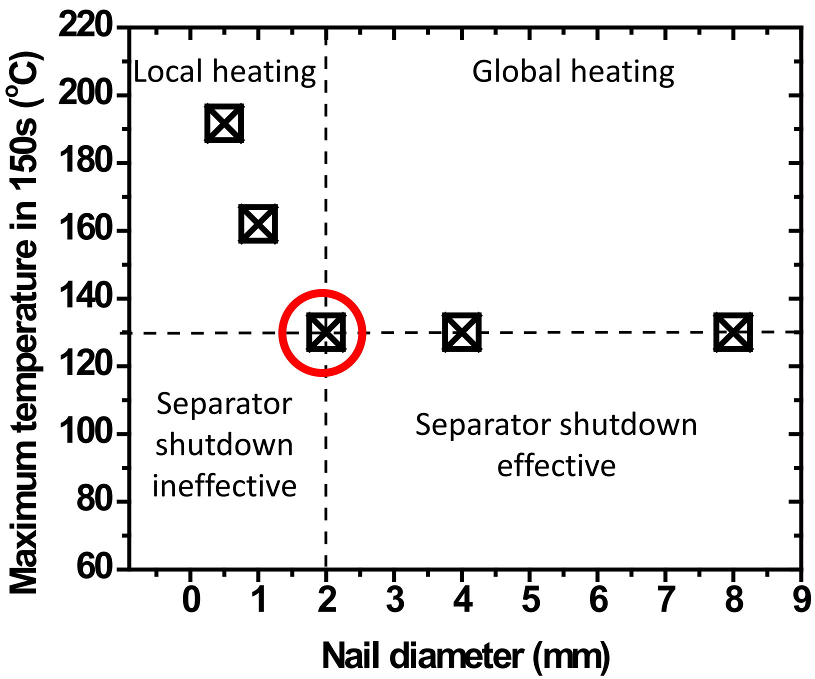
Diameter = 8 mm

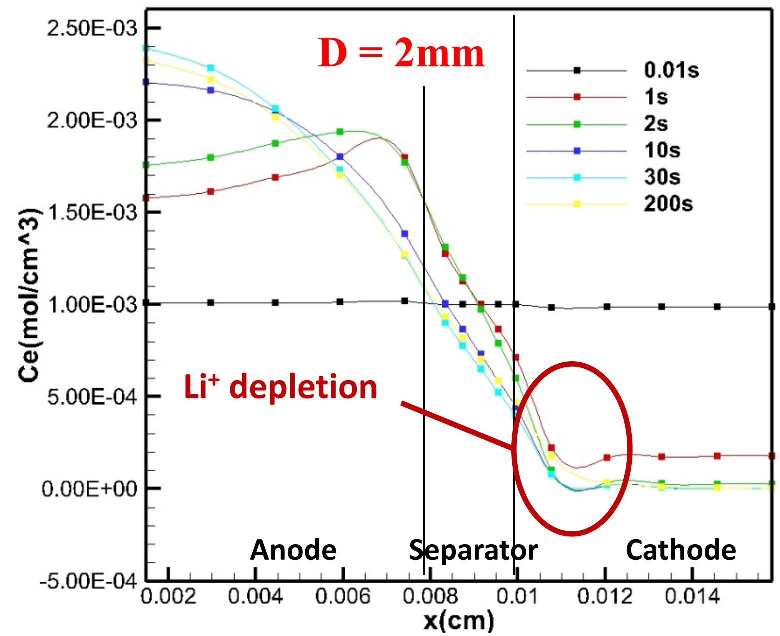


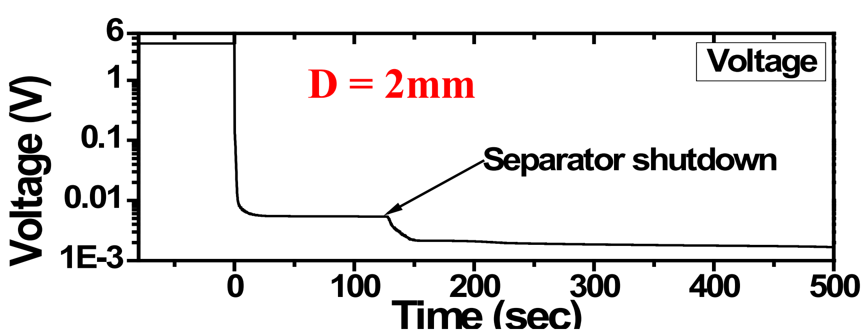
Rapid temperature rise caused by ***electrochemical effects*** (e.g. nail penetration) can only be predicted with ***electrochemical thermal (ECT) coupling***

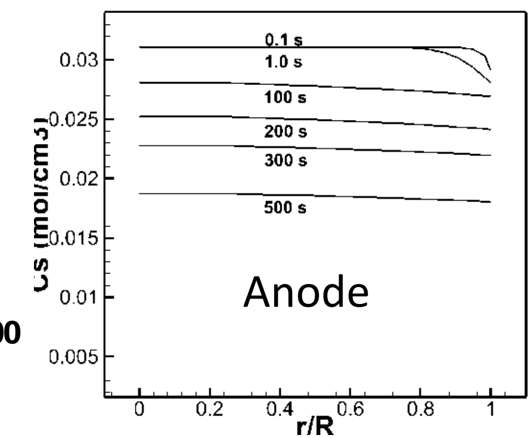
Accomplishments - Safety

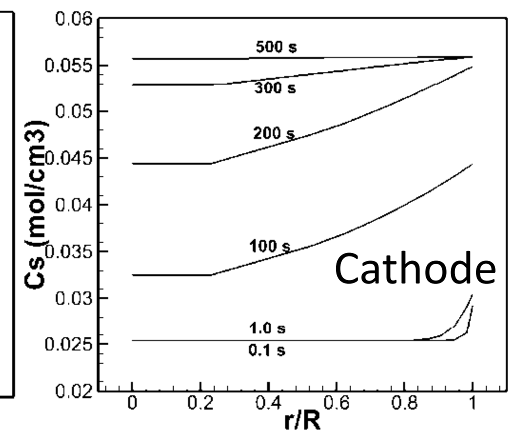
Full Penetration







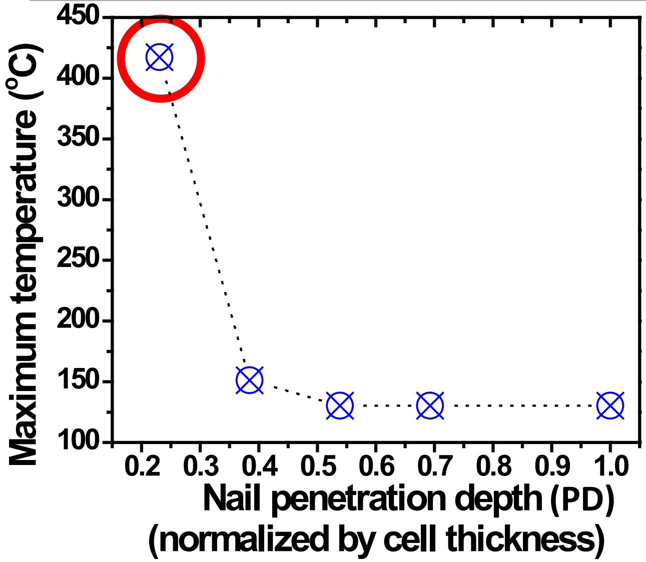




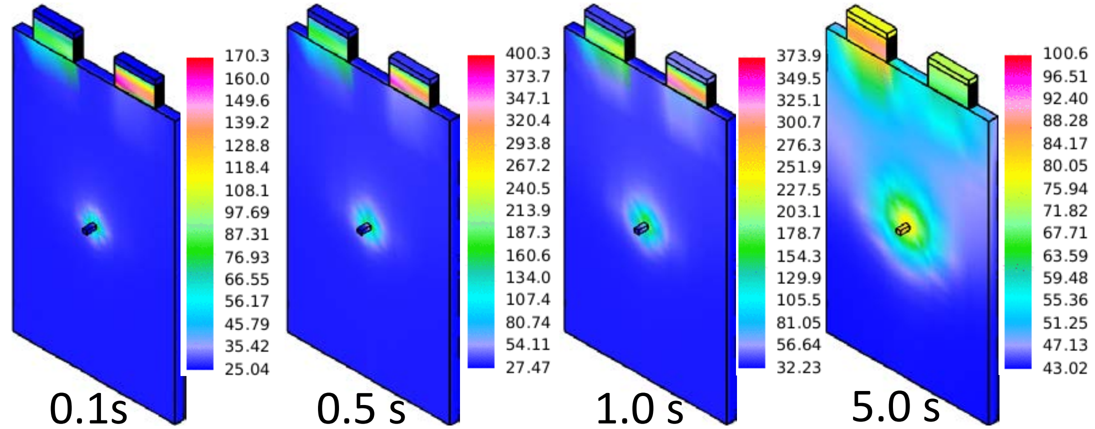
Simultaneous t***hermal and electrochemical*** results during ***safety-related events***

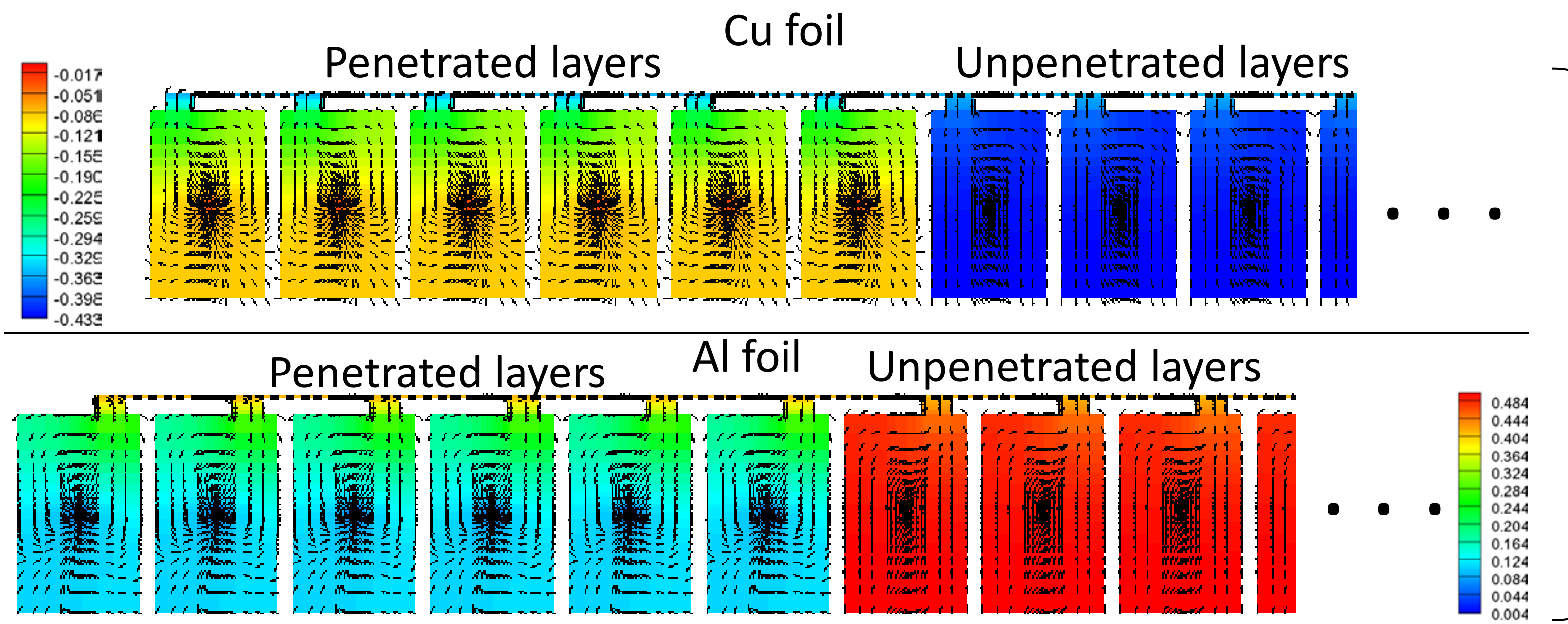
Accomplishments - Safety

Partial Penetration



Temperature (°C) for PD = 0.2

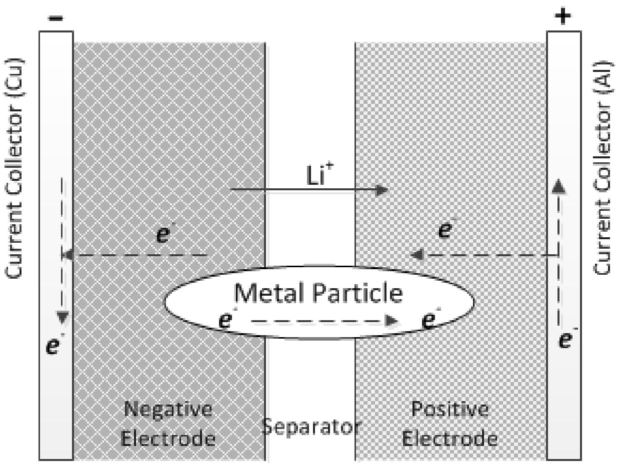


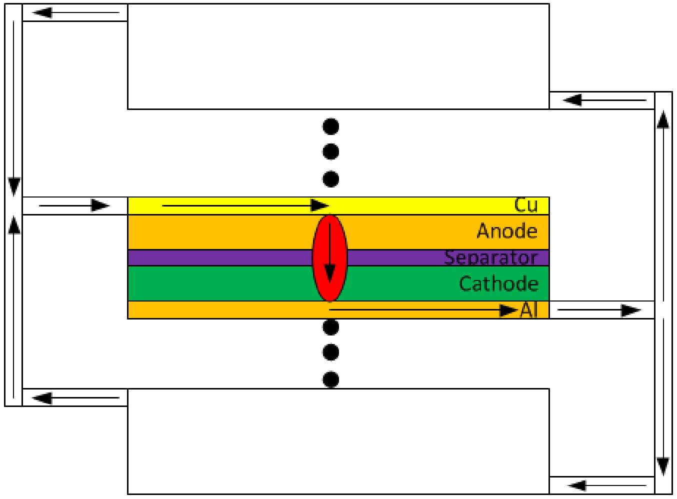


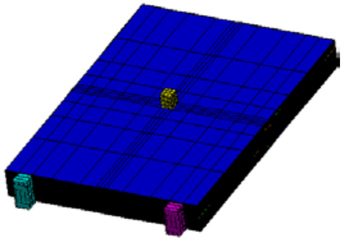
Solid Potential for PD = 0.2

Accomplishments – Safety

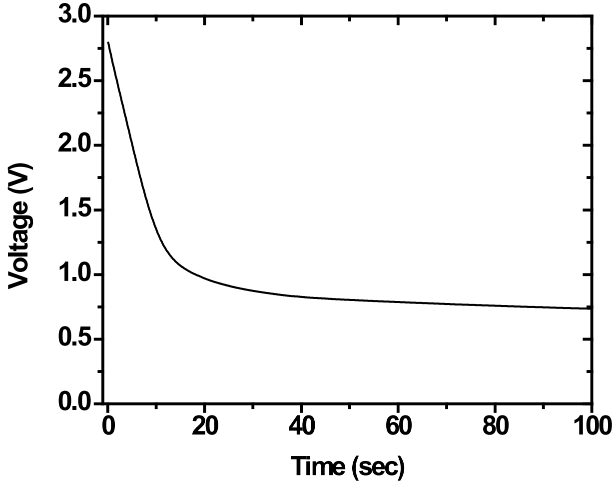
Shorting by Metal Particle

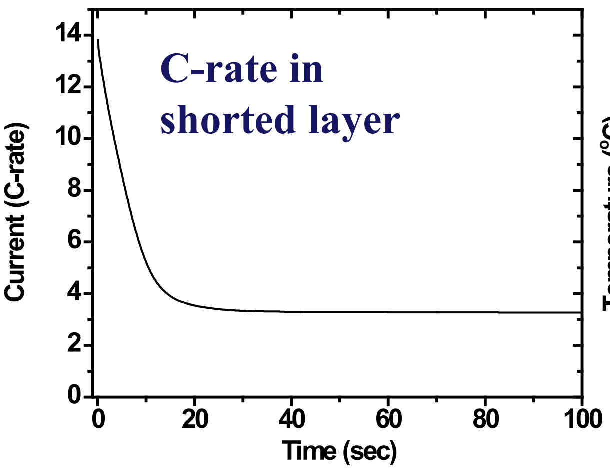


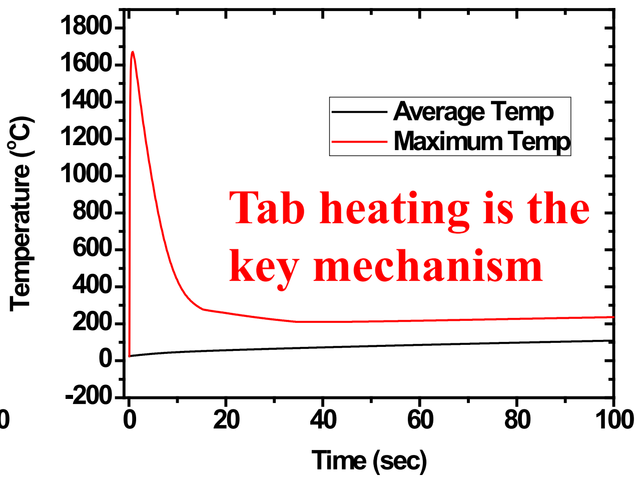




- 10 Ah, 26 layer stacked cell
- $R_{short} = 10m\Omega$
- Short in center of layer
- Short in center layer of stack

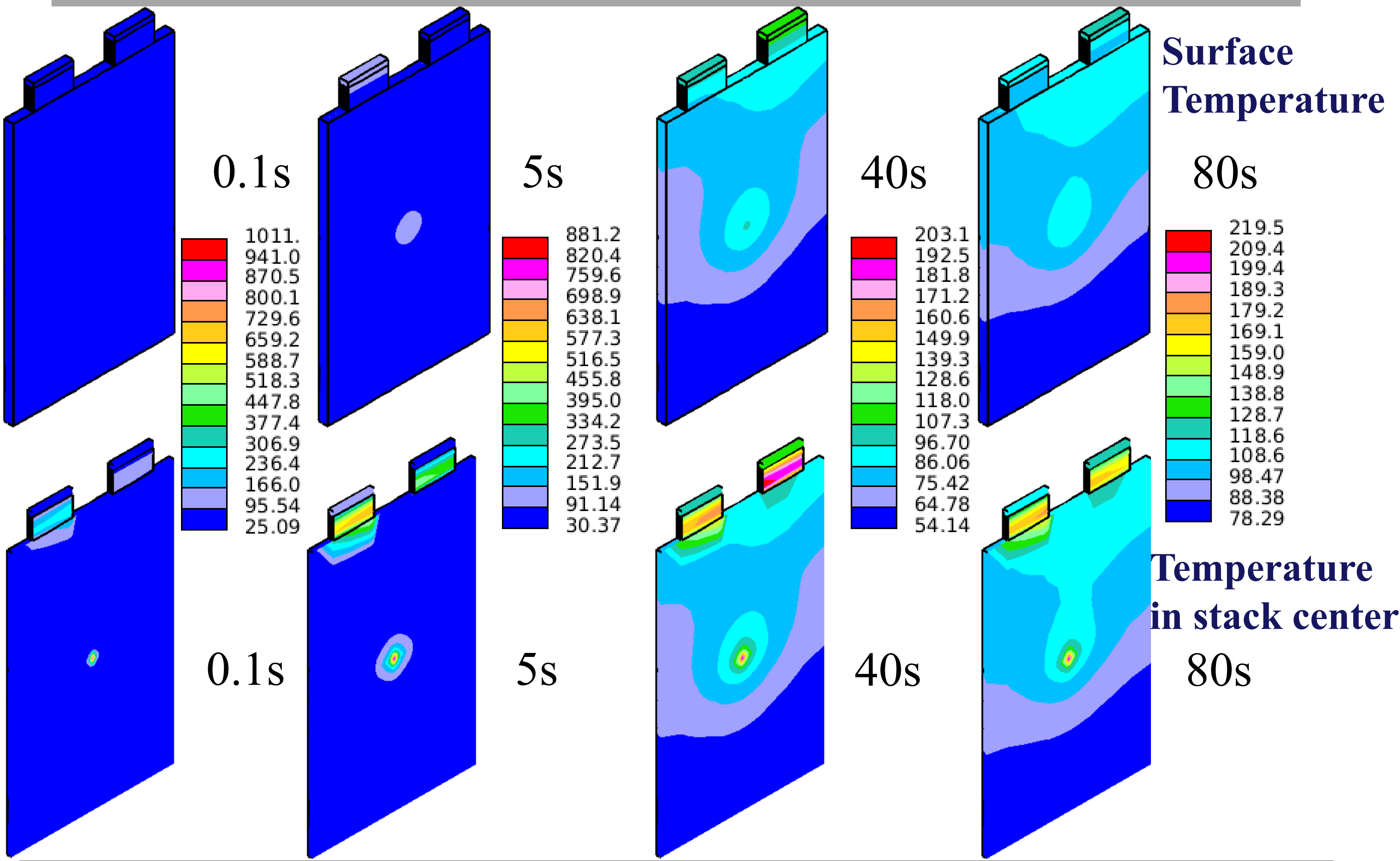






Accomplishments – Safety

Shorting by Metal Particle



Heating greatest in ***tabs*** and in ***metal particle***

Collaboration w/Other Institutions

Funding Agency

CAEBAT Program Administrator

Open Architecture Software

Project Lead – Software development and sales, project administration.

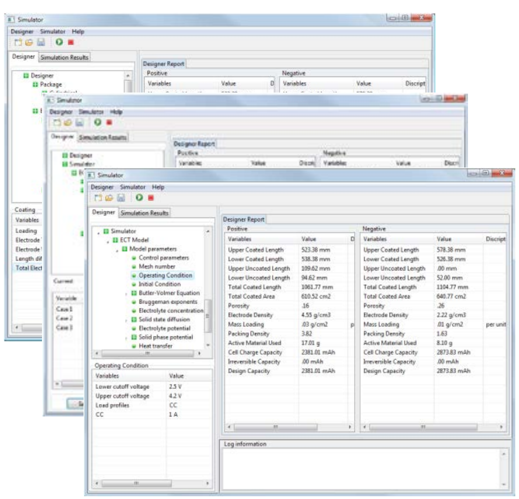
Industrial Partner – testing, validation, and feedback

Industrial Partner – testing, validation, and feedback

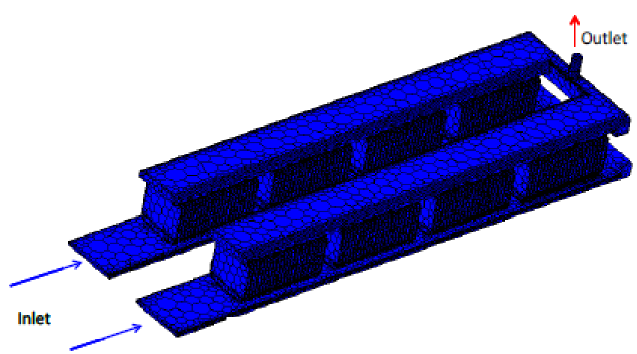
Academic Partner – materials testing and detailed model validation

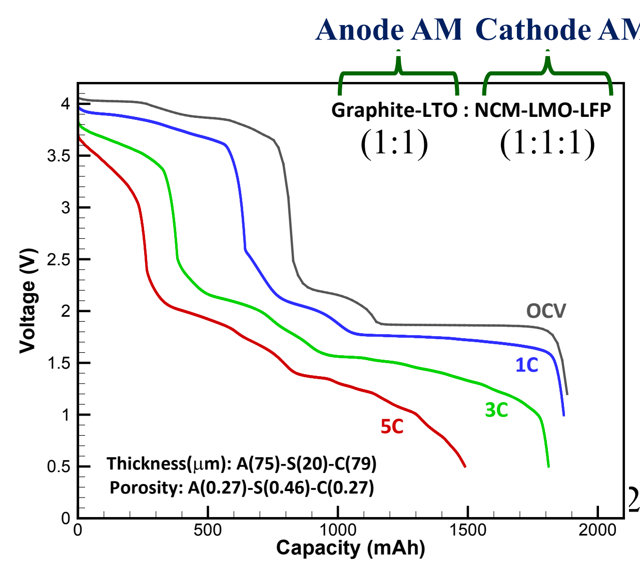
Future Work

- More safety simulation of interest to Ford & JCI
- Pack modeling with electrochemical-thermal coupling
- Further and extensive cell and pack validation
- Refined user interfaces
- Life/degradation modeling; optimization of battery usage
- Additional content for materials database
- Blended electrode models (anode & cathode)
- Quarterly review meetings with all team members



Input and design properties GUI





Summary

- Good progress in 2011
  - Cell level software development
  - Performance modeling on cell level
  - Preliminary safety modeling of cells
  - Materials database
- Commercial partners (Ford, JCI)
  - Began testing ECT3D in December, 2011
  - Will give expanded feedback during 2012
  - ECT3D is a tool to help
    - ***Reduce cost***, "… by accelerating design processes and system optimization using virtual test bench (software)."
    - ***Improve safety***, "… by understanding the benefits and tradeoffs of various safety technologies."
    - ***Improved thermal performances***, "… leading to either cost savings or better life."
- Meeting CAEBAT/DOE goals
  - Helping to accelerate the adoption of automotive Li-ion battery cells & packs
  - Enabling technology for EV, PHEV