Efficient Safety and Degradation Modeling of Automotive Li-ion Cells and Pack

Christian Shaffer (PI)

EC Power

http://www.ecpowergroup.com

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Project ID #
ES200

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Overview

Timeline

- Start date: 10/1/2013
- End date: 9/30/2015
- Project 25% complete

Barriers

- Barriers addressed
  - LiB Safety/Abuse
  - LiB Lifetime
  - LiB Efficiency
  - Computer tools for design exploration

Budget

- Total project funding: $2.0M
  - $1.0M (DOE)
  - $1.0M (cost share)
  - Fed. cost through 12/31/13: $134.5 k

Partners

- Penn State

Funding provided by **Dave Howell** of the DOE Vehicle Technologies Program .
The activity is managed by **Brian Cunningham** of Vehicle Technologies,
through NETL, **Bruce Mixer** Technical Monitor

Project Objectives - Relevance

- Develop an efficient & robust pack-level safety and abuse model
  - Predictive tool with electrochemical-thermal (ECT) coupling
  - Virtual tool to assess/screen safety of cell/pack designs
- Develop mechanism-based, fundamental models for accurately predicting degradation of Li-ion batteries
  - Predictive models valid under user-specified and wide-ranging temperatures and operating conditions
- Perform co-simulation of our software with structural mechanics software via the Open Architecture Standard (OAS)
  - Electrochemical-Thermal-Mechanical (ECT-M) coupled simulation
- Perform testing and validate the cell- and pack-level safety and degradation models
- Expand extensive materials database
  - Experimentally characterizing and adding NCA to our database
- Develop commercial software to be used by licensees
- Support DOE CAEBAT activity

Project Milestones & Activities

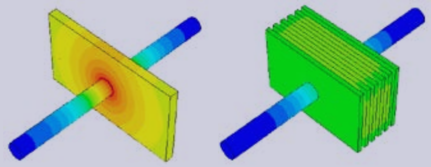
Recent Milestones Completed
M1: Project kickoff; all agreements and sub-agreements executed
M2: Completion of initial model development for safety, abuse, and life

Milestones in Progress
M3: Complete fabrication of large-format cells for safety, abuse, and degradation testing
M4: Safety, abuse, and degradation testing 50% complete
M5: Materials database characterization 50% complete
M6: Initial model implementation complete for safety, abuse and degradation
Budget period #1 Exit (12/31/14): Go/No-Go

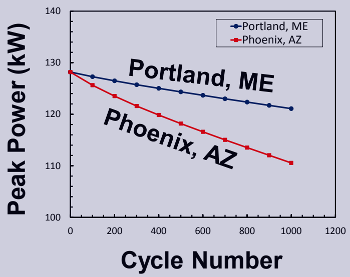
Approach – Supporting CAEBAT Activity

Modeling

Safety/Abuse

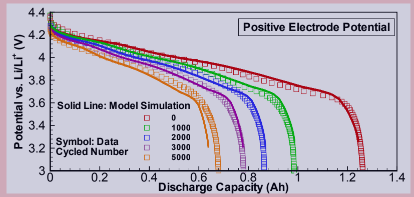


Life

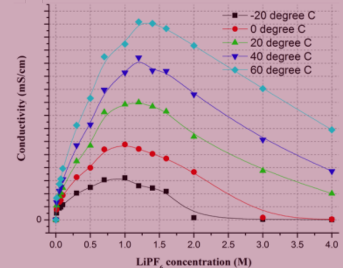


Co-Sim. via OAS (ECT-M)

Validation



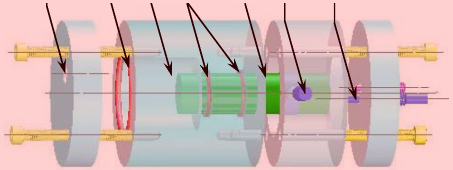
Materials Database



Experimental

Safety Testing

Life Testing

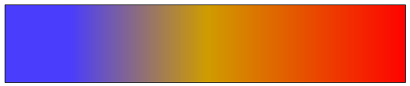


Materials Char.

*End Product: **<u>Experimentally validated</u> <u>commercial tool</u>** with advanced **<u>safety/abuse and life models</u>**, along with **<u>commercially-relevant materials database</u>***

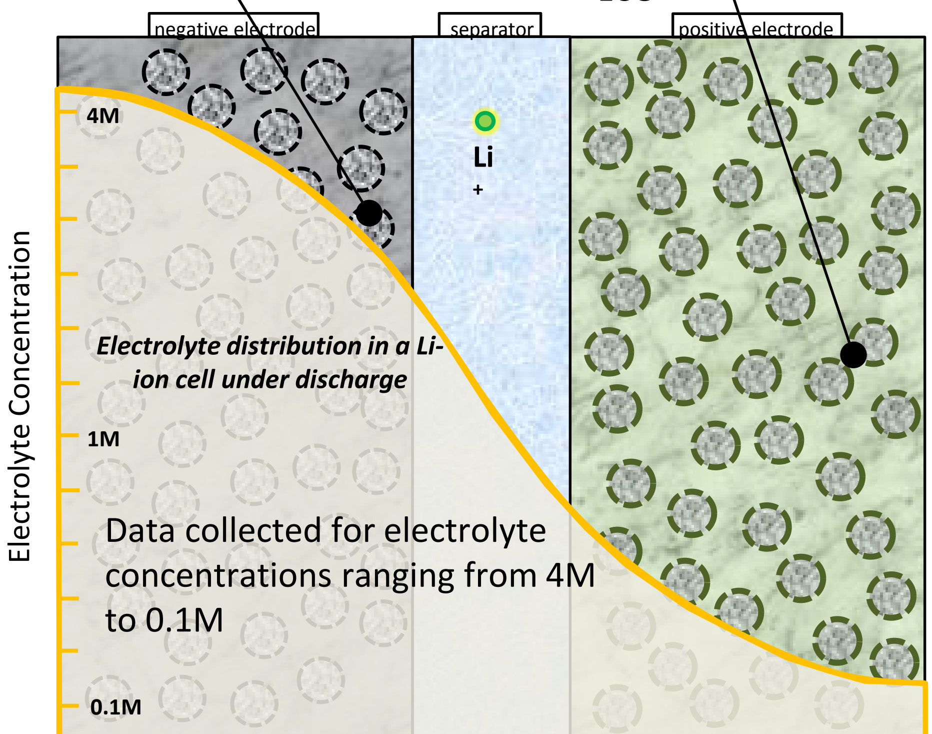
Approach – Materials Database

Tested temperature range for materials

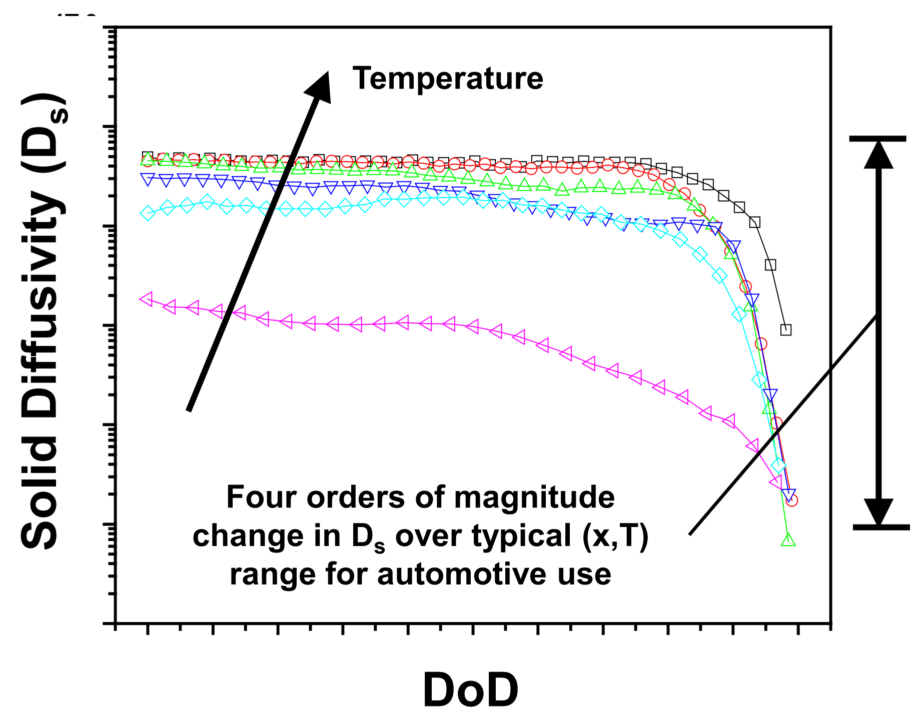
-30°C  100°C

Existing Anode Materials:
- Graphite (blend natural/syn.)
- LTO

Existing Cathode materials:
- NCM
- LFP
- LMO
- LCO



Adding NCA as part of this project
- GITT for $D_s = f(T,x)$ and $OCP = f(T,x)$
- EIS for $i_o = f(T,x,c_e)$



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 Modeling

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
  - Safety simulations
  - Thermal runaway
  - High power, low-T operation
  - Heating from subzero environment

Accomplishments – Materials Database

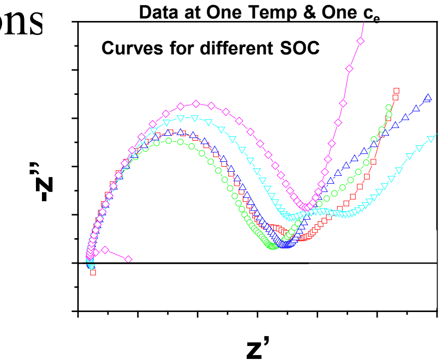
NCA Property Measurement

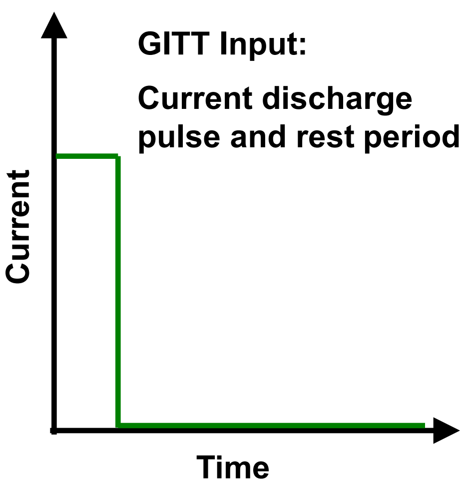
GITT Test – OCP and Ds

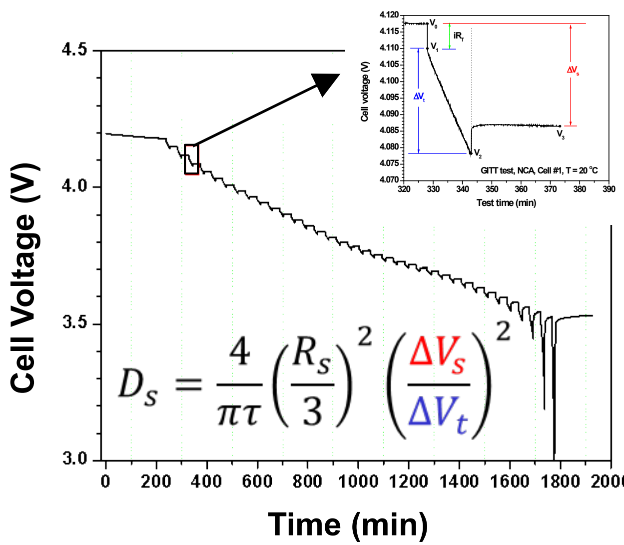
- To get OCP = f(x,T) and D_s = f(x,T)
- 6-8 months to carry out full matrix of (x,T) combinations
- At one T, 40+ data points to get data for entire (0 < SOC < 1) range
- NCA/Li half cells used
- Nearly complete

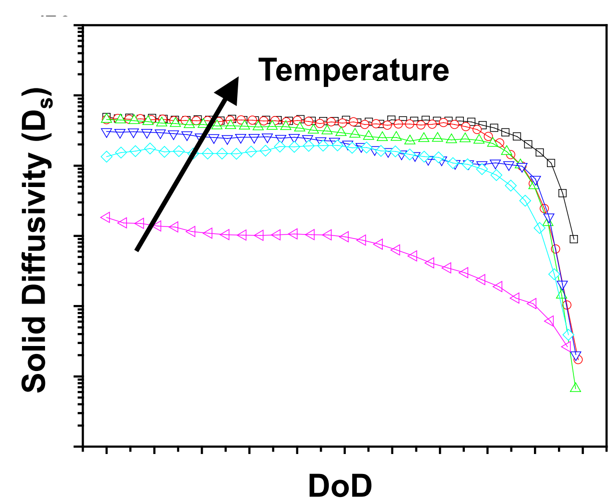
EIS – Exchange Current Density

- To get OCP = f(x,T) and D_s = f(x,T)
- 6-8 months to carry out full matrix of (x,c_e,T) combinations
- NCA/Li half cells
- Recently started





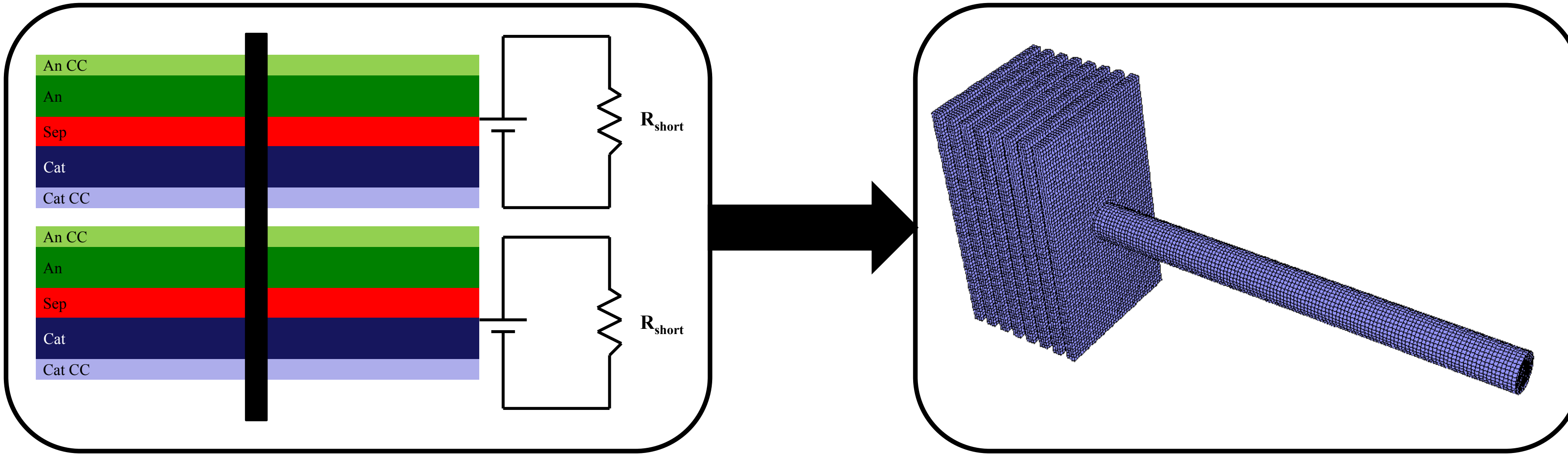




*Adding **NCA properties** to **materials database** for accurate Li-ion battery prediction under **automotive conditions***

Accomplishments – Pack-level Safety

Initial Implementation of Pack-level Shorting Model



- We have developed a robust approach and algorithms to efficiently simulate nail penetration of multi-cell packs
- Typical nail penetration simulation takes a few hours for one processor per cell (coupled ECT simulation)
- Goal: develop a software that can reliably asses safety of any cell or pack and evaluate effectiveness of various mitigation strategies
  - Nail type, nail size
  - Cell material types, electrode design, capacity, cell/pack geometry
  - Evaluate proposed safety mechanisms under different safety conditions

*The **coupled thermal and electrochemical response** of **pack-level shorting** is captured with the model implemented, in an efficient manner*

Accomplishments – Pack-level Safety

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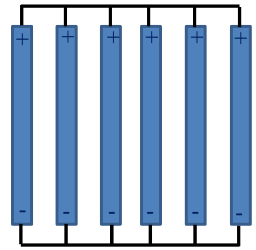
Number and Arrangement of Cells in Pack (1/2)

Case #1

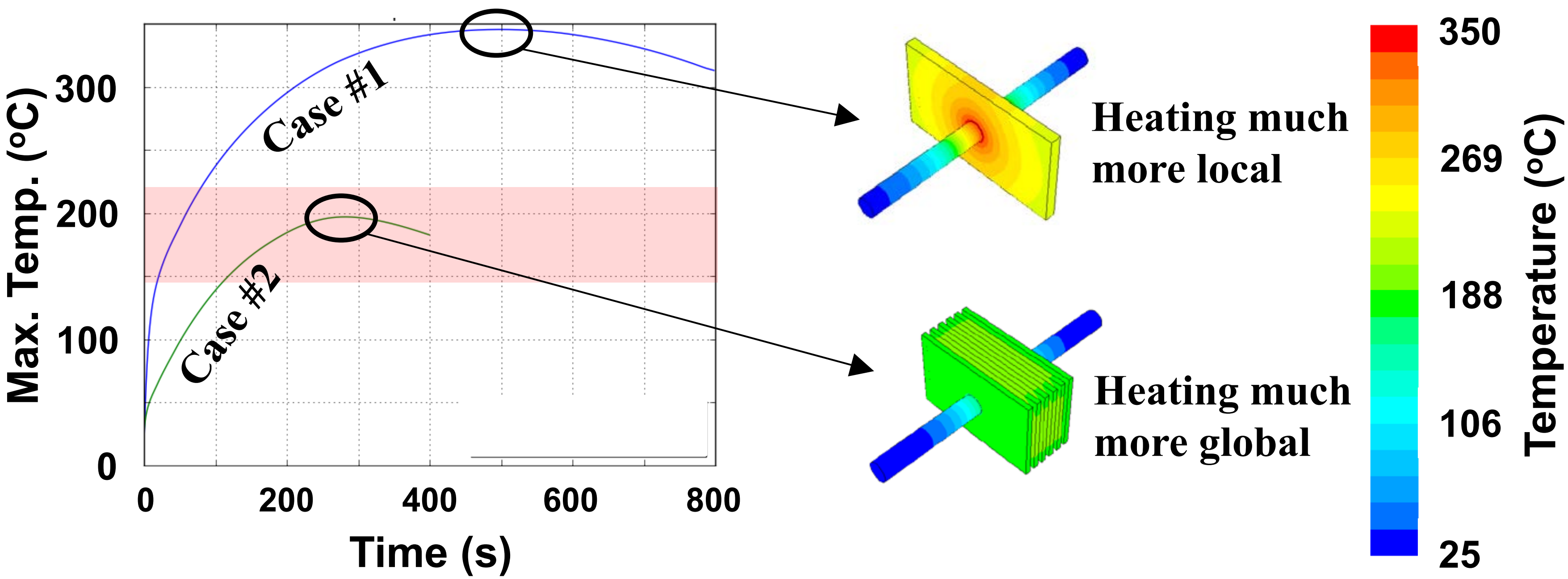
- One 30Ah NMC/graphite cell



Case #2

- 6p/1s configuration of 5Ah NMC/graphite cells

- The two cases are identical electronically (same V, same total capacity)
- Both are shorted by 20mm diameter stainless steel nail
- The 6p/1s arrangement is substantially safer due to more global heating

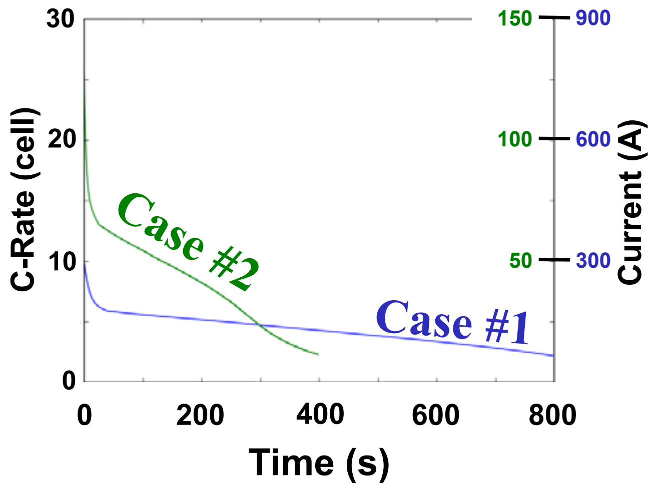


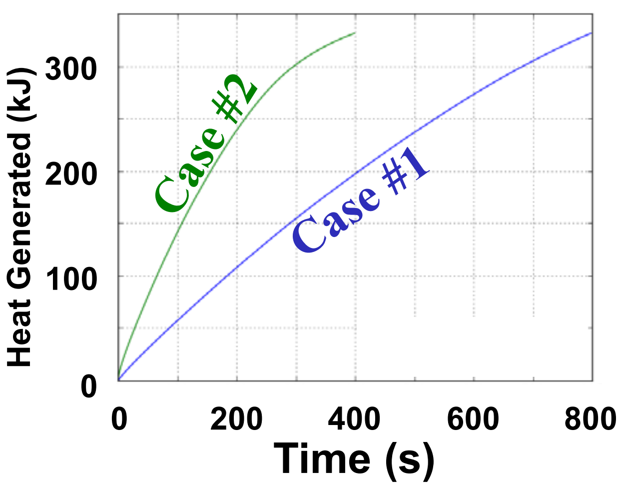
Kalupson et al., ECS Spring Conference, Orlando, FL April 11-15, 2014

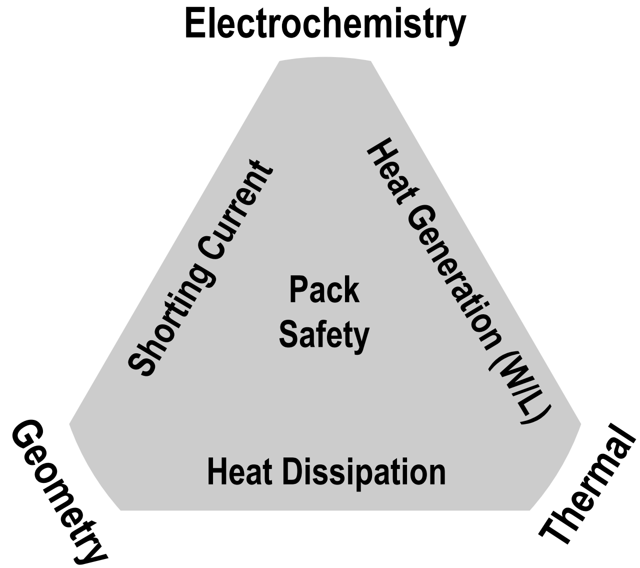
Software used to rapidly and cost effectively assess safety of cell and pack design

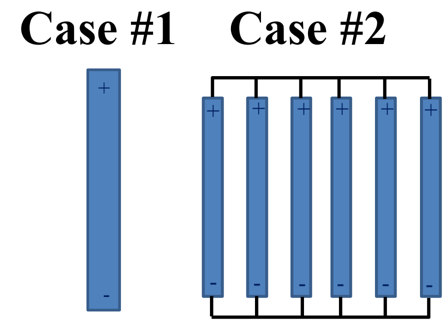
Accomplishments – Pack-level Safety

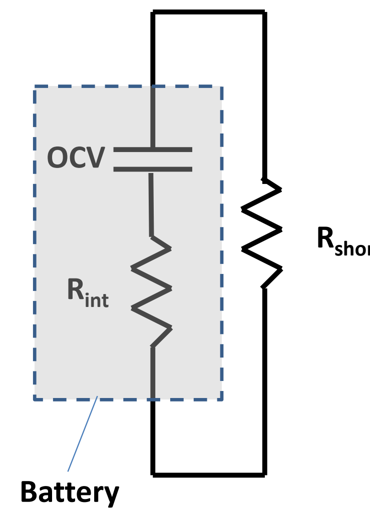
Number and Arrangement of Cells in Pack (2/2)

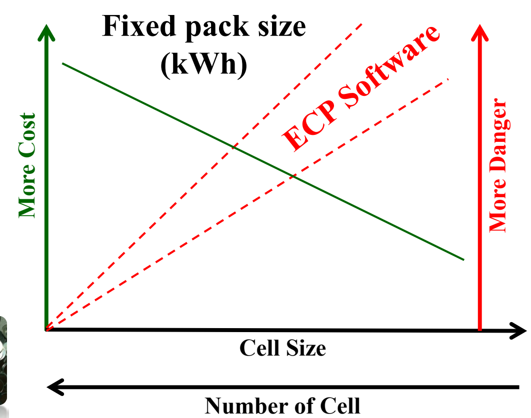


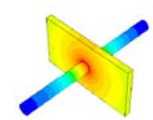










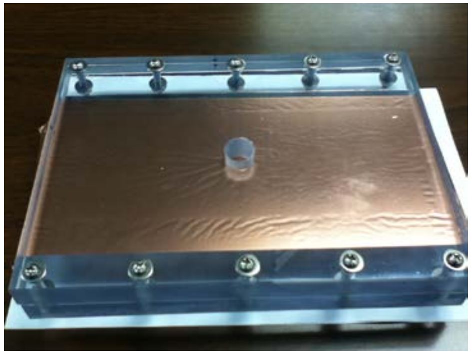


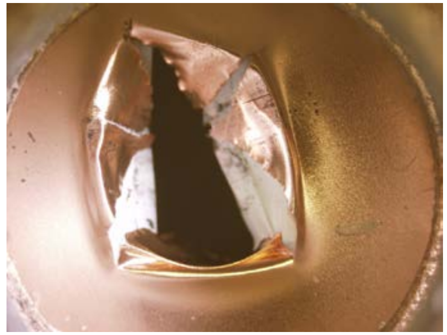
Kalupson et al., ECS Spring Conference, Orlando, FL April 11-15, 2014

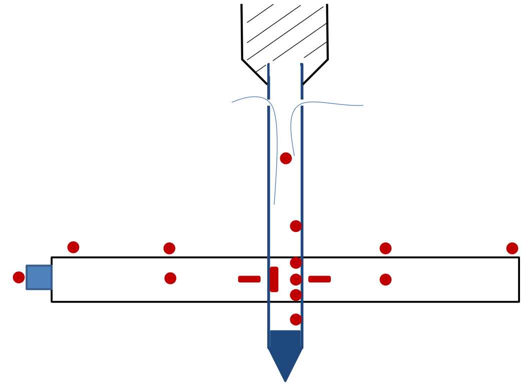
***Pack safety** is dictated by **complex interplay** between **electrochemical, thermal, and geometric factors;** safety can only be determined by models that account for all three factors*

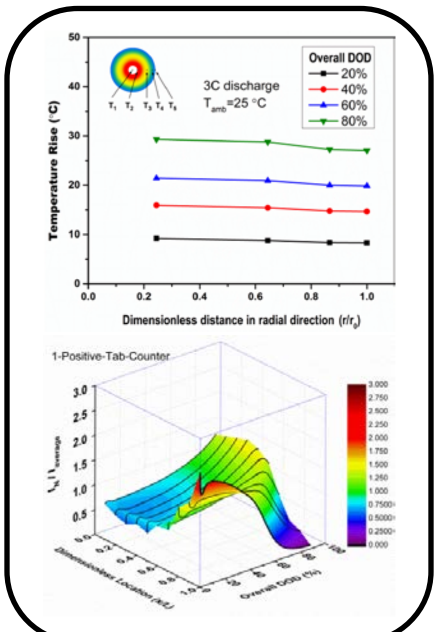
Accomplishments – Safety Validation

Preliminary Nail Penetration Testing









Successful in-situ measurement of temp & current from past work

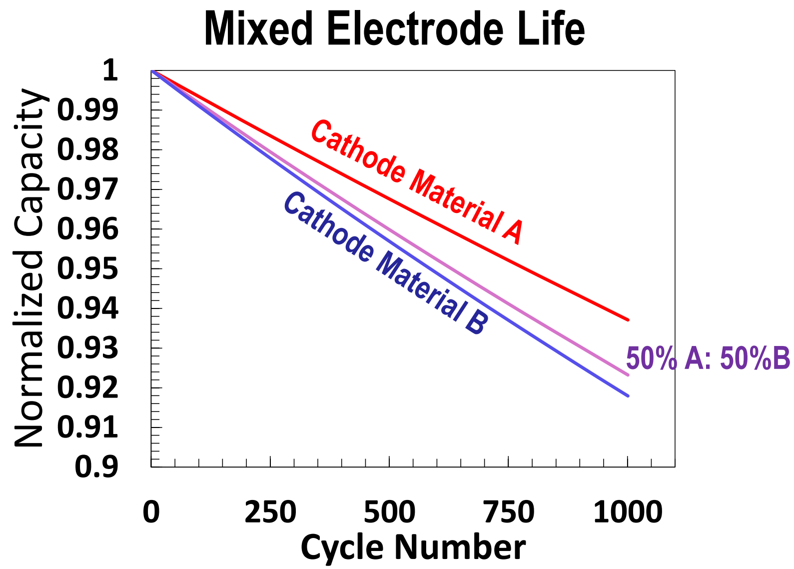
- Goal: measurement of detailed electrochemical and thermal response during nail penetration test (not just temperature)
  - Current and/or contact resistance
  - Multiple sensors embedded in nail and/or cell to validate ECT model
- To date: preliminary testing of various designs
  - Will down-select best designs for future use
- In year two – also perform nail penetration of multi-cell pack (pack-level validation)

Innovative nail/cell design to validate model ECT response of cell /pack during nail penetration process

Accomplishments – Life & Abuse

- Enhanced life and abuse models – completed initial model development (model equations)
  - Enhanced electrode pulverization model
  - Enhanced SEI growth model, including effects of electrolyte additives
  - Life model for user-defined mixed electrodes
  - Overcharge model

Electrode Pulverization



- Currently working on implementing these refined models
- All models are mechanism-based, temperature-dependent, predictive models, i.e. non-empirical

Enhanced models for more accurate prediction of life and features to expand usefulness (e.g. mixed electrode with life)

Collaboration w/Other Institutions

Funding Agency

Administrator

Open Architecture Software

Project Lead – Software development and sales, project administration.

Academic Partner – materials testing and detailed model validation

Future Work

- Complete NCA characterization
- Carry out nail penetration testing and validation
  - Single cell
  - Multi-cell pack
- Continue implementation and validation of enhanced models for life and abuse
  - Accelerated life testing
  - Overcharge testing
- Add additional features to pack-level safety model
  - Add capability to simulate partial penetration of pack (e.g. 3/16 cells shorted) for parallel configuration
- OAS: co-simulation with structural mechanics software (ECT-M simulation)
- These activities reflected in future milestones

Response to Previous Year Review

- This is the first year for this project (no review from last year)

Summary

- Project on track
  - Demonstrated simulation of pack-level nail penetration
  - NCA characterization ongoing
  - Nail penetration testing with innovative approach to acquire data for validation
  - Initial model development complete for enhanced life and abuse models
- Future work tied to milestones and addresses project objectives
  - Completing ongoing tasks
  - Implementation of models developed
  - Validation of safety and life models
  - OAS
- Software is commercially available
- Meeting CAEBAT/DOE goals
  - Helping to accelerate the adoption of automotive Li-ion batteries by addressing barriers to adoption (e.g. life and safety)
  - Enabling technology for EV, PHEV