Coupling of Mechanical Behavior of Lithium Ion Cells to Electrochemical-Thermal (ECT) Models for Battery Crush

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Introduction

- Battery performance, cost, and safety need to be further improved
- Modeling/design tools play important roles to achieve these goals
- DOE CAEBAT-1 activity has resulted in ECT CAE simulation tools

- In CAEBAT-2, mechanical modeling is being added to ECT tools to simulate cell response after a crash-induced crush
Battery MECT Modeling After Crash

• Vehicle crash $\rightarrow$ battery crush $\rightarrow$ cell damaged zone $\rightarrow$ separator failure $\rightarrow$ electrode contact $\rightarrow$ local short $\rightarrow$ current flow $\rightarrow$ heat generation $\rightarrow$ insufficient heat rejection $\rightarrow$ temperature increase $\rightarrow$ onset temperature reached $\rightarrow$ spontaneous reactions $\rightarrow$ thermal runaway $\rightarrow$ smoke and fire

$\rightarrow$: may lead to (depending on many factors)

• Simulating all physics and geometries at the same time is challenging and takes a lot of efforts; simplifications are needed

• Our approach:
  o Decouple structural behavior from ECT interactions
  o Simplify and use **LS Dyna** to simulate structural changes after crush
    - Need to obtain structural/mechanical material properties of cell components
  o Then, capture characteristics of damaged zone and transfer to ECT
  o Finally, use data for electrochemical and thermal modeling
As crash-induced mechanical crush is a much faster process than electrochemical and thermal response, our initial approach was to develop a **sequential one-way coupled** modeling approach.

Conducted electrochemical and thermal modeling on top of a mechanically-deformed geometry.

**Effective Medium Model**

**Recommendations for Material Design**

**Component Properties**

**Object indentation**

**Component level information used to build a constitutive cell-model**
MECT Model: Mechanical Properties Measurements

- Measured mechanical properties of individual components
- Digital Image Correlation (DIC) assisted tensile tests

Anode current collector
Separator
Cathode current collector

MIT Mechanical Characterization

- MIT providing experimental and model inputs, to support the mechanical constitutive and fracture modeling of battery cell components

**Micro testing of collectors**

![Image of micro testing](image-url)

CT images of cell fracture

![CT images](image-url)

Fracture modeling

![Fracture models](image-url)
Component Testing: Tensile Test Results

- Tensile tests showed a typical elasto-plastic response for metallic thin films for the current collectors.
- Anisotropic behavior was observed in the separator tests.


**Electrodes and current collectors**

- Anode
  - Copper foil
  - Al foil

- Anode (coated on copper foil)
- Cathode (coated on aluminum foil)

**Electrodes and separators**

- Separator MD
  - Aluminum Foil Rolling Direction
  - Copper Foil Rolling Direction
  - Aluminum Foil 90R Direction
  - Copper Foil 90R Direction
- Cathode (LiCoO2 on Aluminum) 90R Direction

- Separator TD
  - Aluminum 90 D
  - Copper 90 D
  - Cathode Rolling D
  - Cathode 90 D

**Separator MD**

**Separator TD**
NREL Multi-scale Simultaneously Coupled MECT Model

Macro-scale 3D homogenized mechanical-thermal model

Meso-scale quasi-3D mechanical-thermal model

Pseudo 2D electrochemical-thermal model

Element of the macro-scale model

\[ d\bar{\varepsilon}, dt, t, T \]

\[ \bar{\sigma}, \sigma_i, \bar{\varepsilon}, \varepsilon_i, T' \]

\[ R_{\text{short}}, K_{S_i}, dt', t', T' \]

Temperature is assumed to be uniform across each LSDYNA macro element. And the temperature rise is calculated based on the generation of joule heating energy and electrochemical reaction heats.

\[ R_{\text{short}} = A_{\text{short}} \sum \frac{1}{\kappa_s^{(i)}} \]

• Short Resistance (Ω•m³)

Different type of shorts can be distinguished by the short area for the different failure modes of separator layer, e.g. tensile failure or shear failure.

• Temperature

Temperature is assumed to be uniform across each LSDYNA macro element. And the temperature rise is calculated based on the generation of joule heating energy and electrochemical reaction heats.
• Linear elastic mechanical response for electrodes and separator were used for demonstration purposes.
• Strain based failure criteria for separator was used to simulate short-circuit.
• The current shows an instant increase and then starts drop due to the decrease in the cell voltage.

Simulation Conditions:
• 5 Ah LiCoO₂/graphite cell
• The cell voltage of fully discharged is set to 2.8V and the battery model stops after that.
• The model uses 2 minutes for 10⁶ time steps.
NREL Numerical Study on the Effect of Short Resistance

- The developed MECT model is further utilized here to investigate the effect of short resistance on the battery cell performance.

The model captures the effect of short circuit resistance on the subsequent electrical response.

- With the decrease of short circuit resistance, the instantaneous increase of current and voltage drop increases, the discharging completes in a much quicker manner.

- The temperature profile is consistent with the voltage/current evolution profiles, a lower short-circuit resistance does not always produce a higher temperature: there are trade-offs between the cell’s energy content, how fast it can be dissipated as heat in the electrochemical models versus heat transfer rates away from the point of generation.
ANSYS Integration of Mechanical - ECT Coupling

- ANSYS implementing the developed MECT model in ANSYS products, providing technical supports on the coupling method

- Convenient “vertical app” around standard ANSYS products
- Plug-and-play with other products via open-standard interfaces
SNL Battery Abuse Testing for Validation

- SNL providing experimental abuse test of batteries to support MECT model development

**Module Compression**

- Determining coupled failure behavior of batteries during crush/impact testing
- Providing module level data support for validation of MECT model

**Analog “pole test”**

**CT image of structural failure**
SNL Abuse Testing Planned

- Single cell end crush – new fixture built for single cell tests
- Failure mode investigation - Crush and CT analysis of charged and discharged packs crushed to predetermined displacement
- Dynamic Testing – drop testing at burn site

**Single cell test data**

![Single cell test fixture](image)
Summary

• Developed a material model for simultaneously modeling of mechanical-electrochemical-thermal behavior
• Predicted the electrical short, voltage drop and thermal runaway behaviors followed by a mechanical abuse induced short
• Studied the effect of short resistance on the battery cell performance
• Demonstrating the applicability of the developed model for full pouch cell abuse simulation
• Received first round of data from SNL on abuse test of battery module
• Implementing ABDT tool into standard ANSYS System in Workbench
Future Work

• Full cell numerical study using the material model presented in this report.
• Verification compared with existing electrochemical models, for example, ANSYS MSMD model.
• Evolve ABDT into standard Analysis System in Workbench
• Work with MIT on fracture modeling of battery cell components.
• Validation against test data from SNL.
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