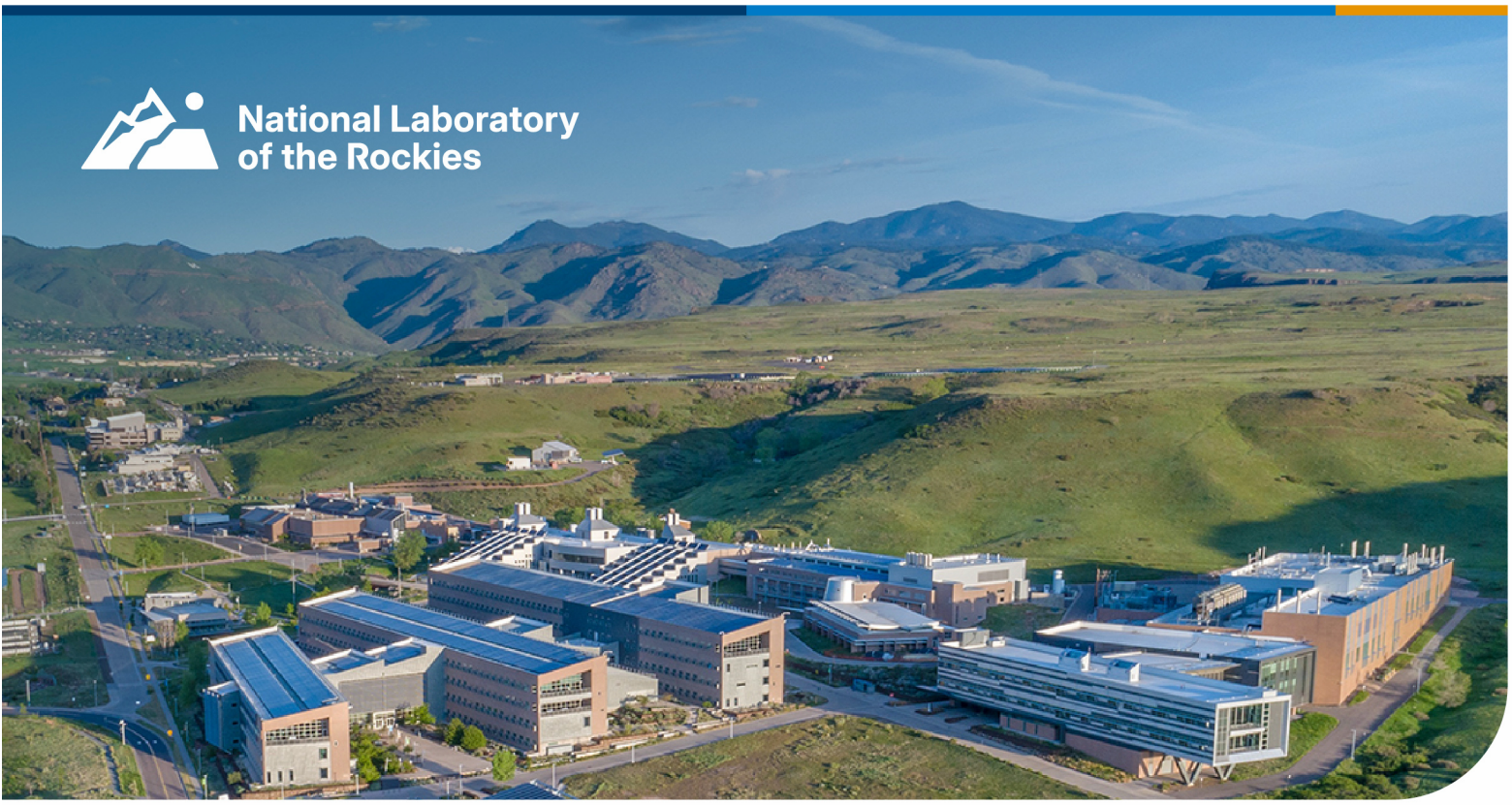

Mechanical, Electrochemical & Thermal Modeling of Electric Vehicle Batteries for Crash Simulation

Cooperative Research and Development Final Report

CRADA Number: CRD-19-00811

NLR Technical Contact: Shriram Santhanagopalan

The National Laboratory of the Rockies is a national laboratory of the U.S. Department of Energy, Office of Critical Minerals and Energy Innovation, operated under Contract No. DE-AC36-08GO28308.

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Technical Report
NLR/TP-5700-100846
August 2026

National Laboratory of the Rockies

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Cooperative Research and Development Final Report

Report Date: May 18, 2026

In accordance with requirements set forth in the terms of the CRADA agreement, this document is the CRADA final report, including a list of subject inventions, to be forwarded to the DOE Office of Scientific and Technical Information as part of the commitment to the public to demonstrate results of federally funded research.

Parties to the Agreement: Hyundai Motor Company

CRADA Number: CRD-19-00811

CRADA Title: Mechanical, Electrochemical & Thermal Modeling of Electric Vehicle Batteries for Crash Simulation

Period of Performance: 9/10/2019 – 2/15/2023

Responsible Technical Contact at NLR:

Shriram Santhanagopalan (no longer at NLR)

Name and Email Address of POC at Company:

Jaeyoung Lim | jytree@hyundai.com

Sponsoring DOE Program Office(s):

Office of Energy Efficiency and Renewable Energy (EERE), Vehicle Technologies Office

Joint Work Statement Funding Table showing DOE commitment:

No NLR Shared Resources

Estimated Costs	NLR Shared Resources a/k/a Government In-Kind
Year 1	$.00
Year 2, Modification #1	$.00
Year 3, Modification #2	$.00
Year 4, Modification #3	$.00
TOTALS	$.00

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Executive Summary of CRADA Work:

Under the proposed effort in partnership with Hyundai Motor Company (HMC), the National Laboratory of the Rockies'(NLR) will cooperate with HMC to develop mathematical models for battery cells and modules for simulating abuse response in batteries subject to the type of mechanical crushing that can occur in a full motor vehicle crash.

CRADA benefit to DOE, Participant, and US Taxpayer:

- Assists laboratory in achieving programmatic scope.
- Enhances the laboratory's core competencies.
- Enhances U.S. competitiveness by utilizing DOE developed intellectual property and/or capabilities.

Summary of Research Results:

WP1. Construct the simulation model (LS-DYNA) for cell level test and compare the test results

Description of the material cards (LS-DYNA MAT) of the cell components. Description of failure model of the cell components. Description of element size and type dependence of cell components. Identify battery modeling approach.

Owing to the complexity of coupling mechanical and electrical solvers for finite element analysis (FEA) of mechanical abuse of a battery, the simulation should be performed by incorporating a local short circuit model activated based on the status of battery elements. However, the approach should also consider various other conditions of the battery simulated, such as the initial state of charge (SOC), for precise simulations of the internal short. This study proposes an approach developed with a mechanical model and single-particle battery model, along with a reaction kinetics model for thermal abuse using LS-DYNA. Several key parameters were selected, such as the activation criteria, kinetic abuse and element integration points during the internal short circuit induced by the indenter. The impact of these key parameters in the FEA on thermal runaway response for various initial SOCs from 25 to 100 % were analyzed. The FEA results obtained were compared against experimental results with various parameters such as activation criterion of internal short, kinetic abuse based on accelerating rate calorimetry (ARC) data. Finally, the root causes of the discrepancy between the FEA and experimental results are discussed regarding integration point what solver can make difference during calculation.

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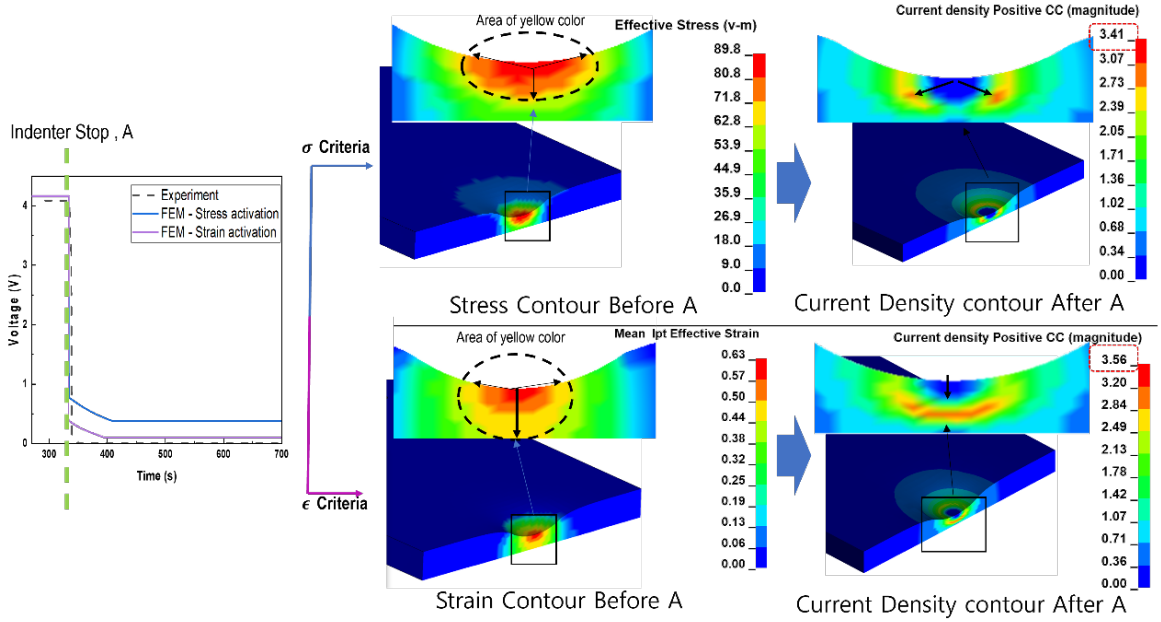

Fig 1: Comparison of numerically predicted and experimental voltage-time responses for two activation criteria (left graph), contour of each criterion before short circuit activation (middle picture) current density contour (right picture) after short circuit activation using stress (right up) and strain (right down) criteria, and comparison of voltage-time responses between FEA and experiments using strain criteria

An activation criterion case study was conducted to determine whether the criterion is appropriate for an SP model. Fig. 1 shows the voltage drop curves for the two activation criterion candidates when the initial SOC was 100. The stress and strain for the criterion were obtained from the FEA when the indenter deformed the same displacement for the internal short circuit in the experiment, as shown in Fig. 1. The curve of Fig. 1 shows that the voltage dropped sharply when strain was used as the activation criterion.

This study proposed and validated a new mechanical–electrochemical–thermal multiphysics model to describe the internal short of a high-capacity cell in FEA. This study simulated the thermal runaway of a high-capacity cell by adding kinetic abuse using a sub-chemical model to the mechanical–electric coupling model. This study mainly focused on the adoption of kinetic abuse obtained from the ARC test and its use of the degree of conversion, α_i, between thermal steps. In addition to the kinetic abuse, additional parameters, such as activation criteria and integration point setting, were proposed to describe the internal short circuit in the battery. The simulation results were validated with experiments. The key results of this study are as follows:

(1) The activation criteria were selected between similar levels of stress and strain such that the best parameter which could describe the short experiment was selected. Effective strain and effective stress were used for the activation criterion that adds a virtual short circuit in a cell. Owing to its highly compressive characteristics of the material, the number of elements in the activation criterion increased more rapidly than those in the stress. This increased the current rapidly, which is similar to the experimental results.

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(2) The kinetic abuse model in the thermal solver, the main concept of this study, was studied. When the electrochemical heat was high owing to the high SOC, it induced an additional chemical reaction. Chemical reaction is the reaction of the SEI film in the battery. This model uses the virtual degree of conversion, in the thermal solver rather than make the SEI film a mesh, so the computation efficiency is significantly improved comparing with conventional approaches. Kinetic abuse occurs using the electrochemical heat produced during voltage change. Moreover, an increase in temperature can be depicted in the FEA with kinetic abuse parameters from the ARC test. The well-matched results show that the thermal runaway heat source from the internal short due to deformation was the same as the battery pouch cell self-heat due to the SEI film.

(3) The integration point must be determined because the LS-DYNA calculates kinetic abuse at the integration point. Irregular thermal propagation and an inverted vertical relationship between TC1 and TC2 were observed with a reduced integrated point. This tendency was opposite to the experimental results. This is because the heat from the reduced integration translates to a higher heat source than that from a fully integrated one. This is because the reduced integration element dealt with the mean temperature at each node. The differences between the reduced and fully integrated systems were significant when the initial SOC was 100, but the difference decreased as the SOC decreased.

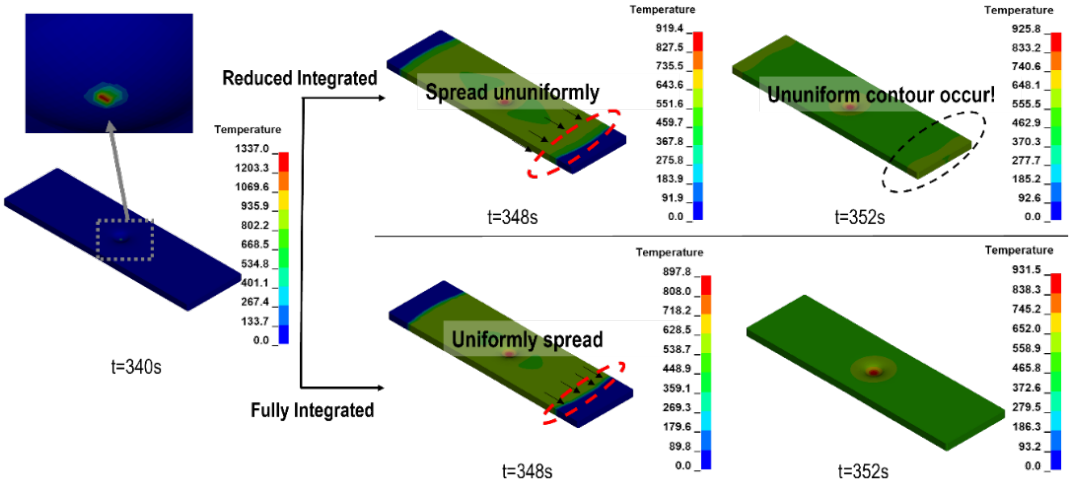

Fig 2. Temperature contour when right after voltage drop(t=340s) and 8,12 seconds after voltage drop (t=348s, 352s) for initial SOC 100

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WP2: Construct the simulation model (LS- DYNA) for module level test

Use cell-level test results (or simulation results from WP2) as input to build finite element modeling techniques for modules for application in pre-existing full vehicle crash simulation models.

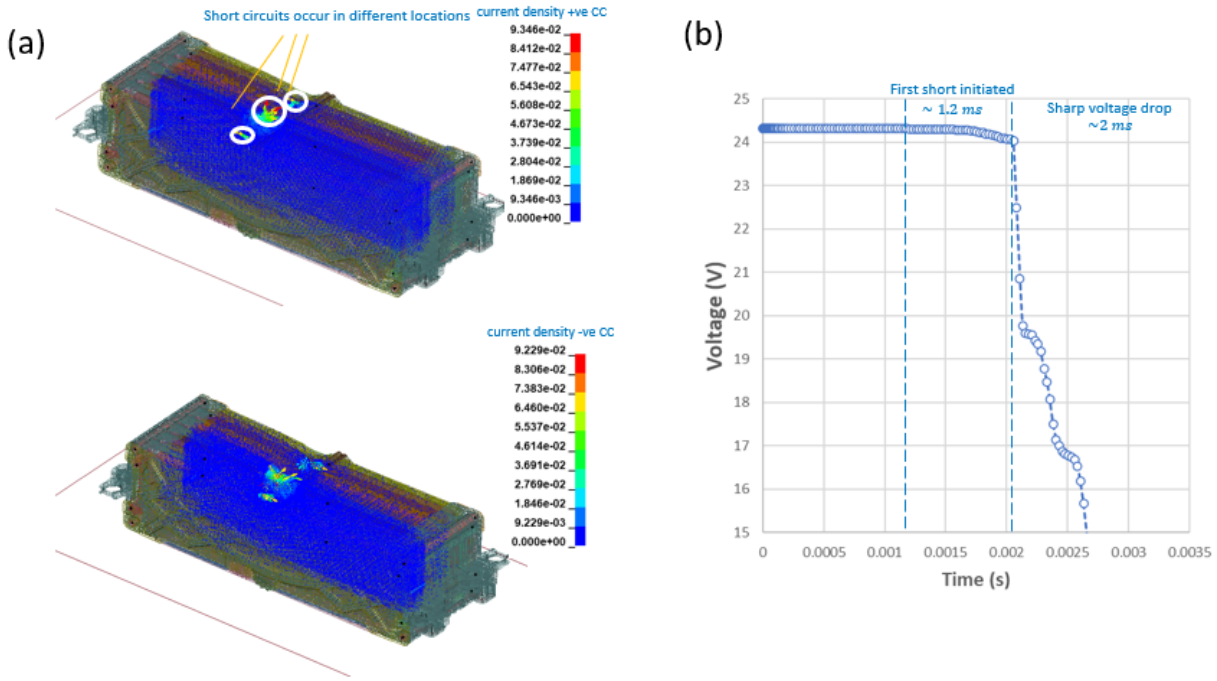

Figure 3. Coupled Multiphysics response upon impact simulation (a) current density in positive and negative current collectors (b) Voltage prediction from multiple internal short circuit instantiations

Developed mechanical model has been extended with methods to simulate internal and external short circuits in battery modules and the simulations were run with coupled mechanical, electrochemical, thermal models. Results indicate voltage starts quickly tapering when the first element shorts at around 1.2 ms. Voltage drops much faster when the second location shorts with a larger contact area. Relatively uniform state of charge is observed during short circuit form impact. All cells experience a soft short whereas current desist profiles are noticeable only in 4 cells. Few milliseconds during the impact do not provide enough time for thermal propagation.

Higher indenter radius initiated short faster. Dependence of voltage on short circuit resistance is as expected and needs to be calibrated to the experiments. Both short circuit initiation strain and short circuit resistance are important to predict the voltage response correctly. Model predicts that no short circuit will occur in orientation 2 and 3 despite having a higher peak force in the mechanical response. This is because jellyroll experiences very low strain as most of the stress is taken by the structural components of the modules. It is necessary to change orientation of modules for the second case or increase the mass of indenter for a short circuit to occur.

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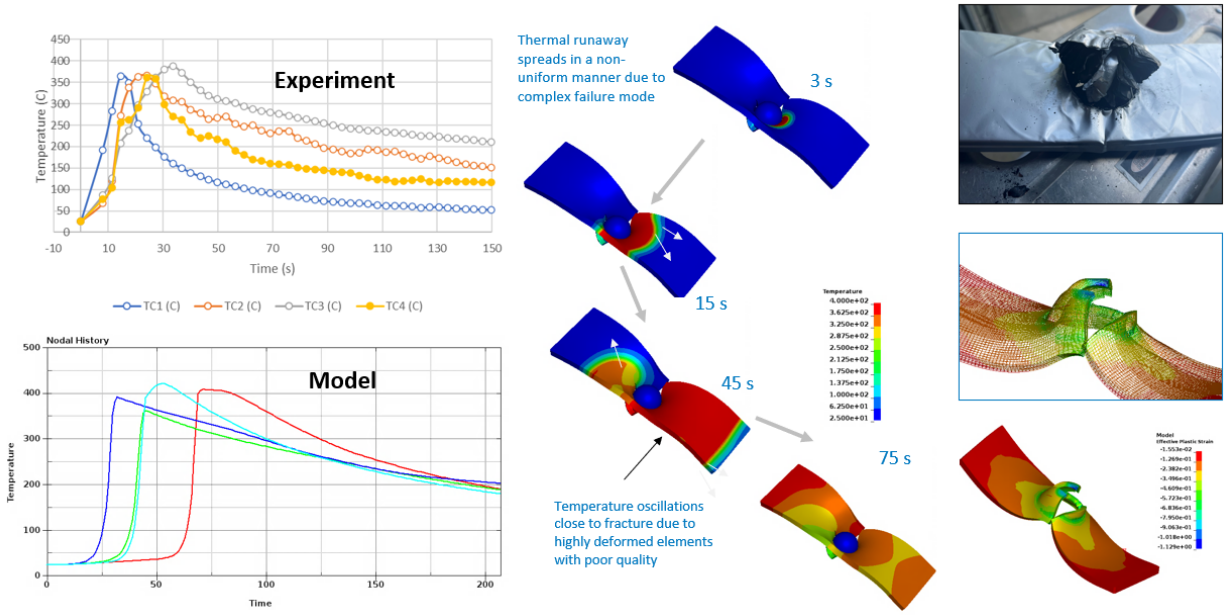

Figure 4: Internal short circuit thermal runaway model results compared with experimental data

Calibrating both voltage and temperature data is extremely difficult based on the initial comparison with models. Model has been improved to include thermally initiated short circuits. This results in a more realistic voltage drop like experimental observations along with thermal propagation results. Comparison of temperature is shown in the figure. Damaged area is quite large in the Through-thickness tests causing significant erosion and distortion.

Overall, module level models with a homogenized jellyroll assumption were completed. Initial velocity of impact is calculated based on drop height and the rigid indenter is gravity loaded to fall onto the module under specified orientations. The battery module deformation and force response is calculated the model using previously obtained material properties from cell level testing. Mechanical only models for RS-RVE can be extended to include electro-chemical and thermal models to better predict the buckling response of the cells. In-plane loading leads to severe buckling in cells which is challenging to capture using a homogenized model.

Modification 3

WP5: NLR will construct the drop test simulation model for modules

HMC will provide test articles* to NLR. NLR will perform cell-level testing. NLR will use cell level test results (or simulation results) as input to build finite element modeling techniques for modules

*All test articles provided to NLR by HMC will be used for destructive characterization and therefore will not be returned to HMC but rather disposed of by NLR.

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There is considerable interest in developing computer aided engineering (CAE) tools to study the response of the batteries. With gasoline-powered conventional vehicles, there are well established CAE tools that simulate various crash response scenarios. However, this knowledge base is still being developed for electric vehicles. Developing models for battery powered vehicles is complicated: besides mechanical and thermal response, we should also consider chemical reactions, high-voltage implications as well as varied length scales and response times for the different physical phenomena. 'Sandwich' level tests for anisotropic modeling were performed in Tension and Compression conditions along with individual components and cell level tests. The cell level mechanical abuse models were correlated with testing data and calibrate the results.

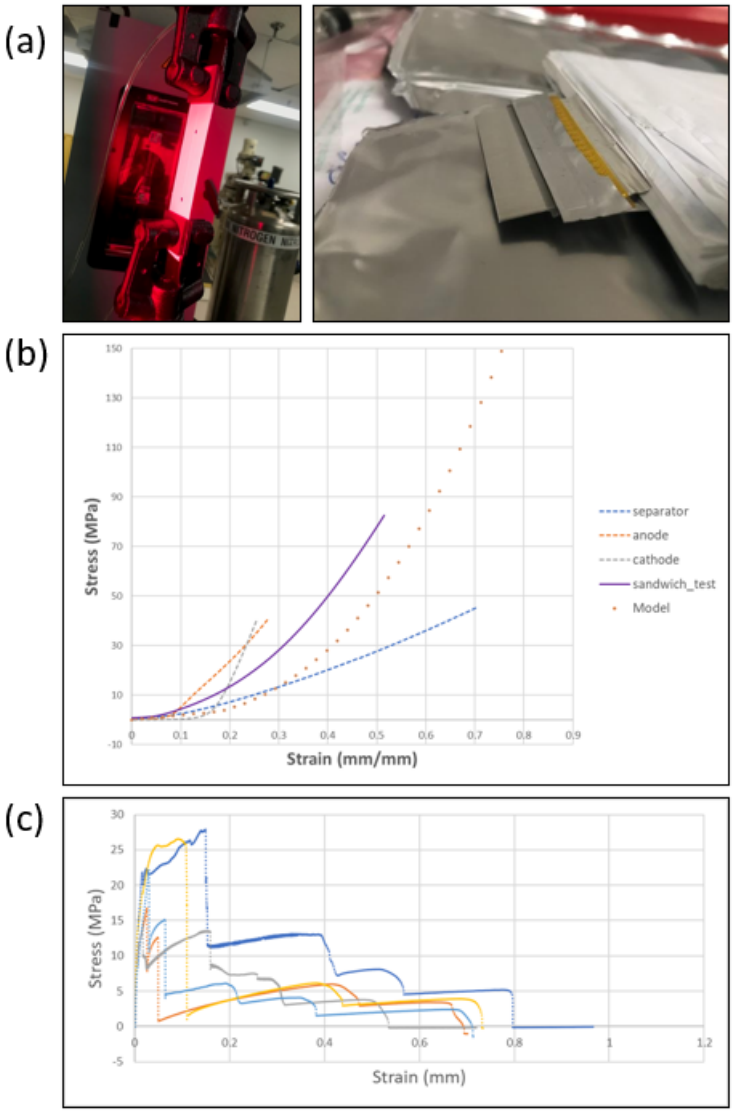

Figure 5. (a) cell and component level testing for extracting mechanical properties (b) compressive behavior of battery components (b) in-plane tensile properties of battery components

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Compression curve of sandwich compared against individual components. Tests are very repeatable with precise response. The composite curve obtained from sandwich tests is slightly stiffer than that obtained from cell level tests. Tension Test is highly stochastic with a wide window for each failure. The regions of failure match the component tests but with increased variance in sandwich level tests. The data is useful for more accurate modeling of failure. These tests provide insights into the anisotropic response of effective jellyroll within pouch format lithium-ion batteries.

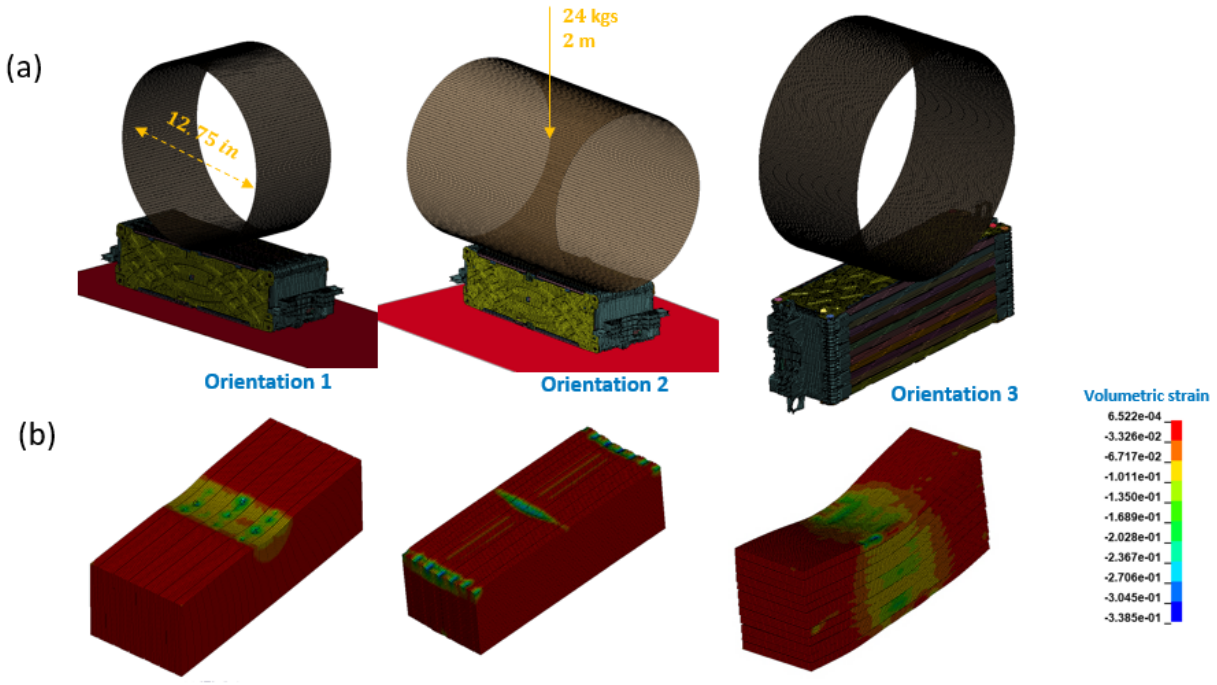

Figure 6. (a) Mesh and input setup for the drop test simulation model for modules (b) strain distribution results obtained upon impact in multiple orientations.

Deformation predicted by using homogenized model shows few eroded elements. Short circuit criterion of effective-stress and element-erosion based are used. Initial simulations indicate that the peak forces on the module will be less than 10 kN in all orientations of impact. From previous experiments, this can mean that the probability of short circuits is low. This suggests increasing mass required in experimental matrix. Using a layered model is possible with minimal modification. This allows for a more realistic buckling mode and prevents overprediction of force.

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WP6. NLR will integrate simultaneous coupling subroutines into LS-DYNA

NLR will work with the LS-DYNA team to integrate NLR subroutines for the electrochemical-thermal simulations on to LS-DYNA software platform. This task requires NLR's coordination with the LS-DYNA team, facilitated by HMC. NLR will support integration on to LS-DYNA to verify functionality.

The schematic below shows how user-defined simultaneous coupling subroutines were integrated into LS-DYNA. The numerical model used for simulation consists of various sub-models that solve corresponding physical processes. Each cell is modeled as a homogenized continuum using solid hexahedral elements. For mechanics, an Isotropic Crushable Foam model (MAT_063 on LS-DYNA) is used for the cells. This model has been used by previous studies for modeling battery deformation and can accurately predict compression behavior. For the purpose of this study, a single particle electrochemical model was selected and implemented using user-defined subroutines within LS-DYNA's BatMac framework. Implementation details regarding coupling with LS-DYNA EM solver and comparison of electrical-thermal responses between electrochemical models have been discussed in a previous paper.

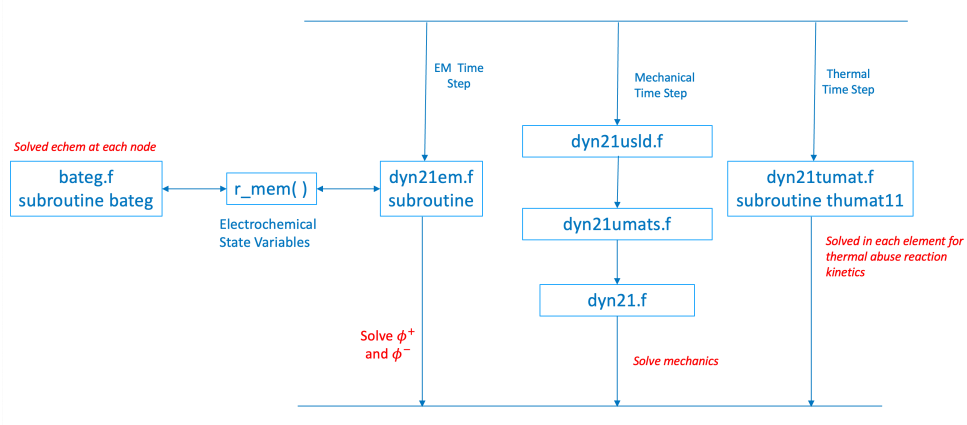

Figure 7. Organization of user defined subroutines and integration with LS-DYNA finite element code.

WP7. NLR will submit the final CRADA Report.

This report serves to meet the requirement for the CRADA Final Report with preparation and submission in accordance with the agreement's Article X.

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Mallarapu, A., Park, S.Y., Lim, J., Han S.B., Lee S.M., Choi, B.H., Han, Y., Sunderlin, N., Santhanagopalan, S. (2025) "Numerical and experimental analysis of mechanically induced failure in electric vehicle battery modules" Journal of Power Sources, 645C (2025) 237245

Park, S.-Y., Mallarapu, A., Kim, J., Santhanagopalan, S., Han, Y., & Choi, B.-H. (2023). Observation and Modeling of the Thermal Runaway of High-Capacity Pouch Cells Due to an Internal Short Induced by an Indenter: Article No. 108518. *Journal of Energy Storage*, *72*(Part C). https://doi.org/10.1016/j.est.2023.108518.

There is no software record directly resulting from the CRADA, but the work has been useful for developing - "SWR-24-100: Coupled Mechanical-Electrical-Thermal Models for Lithium-Ion Batteries"

Subject Inventions Listing: None

ROI#: None

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