Efficient Simulation and Abuse Modeling of Mechanical-Electrochemical-Thermal Phenomena in Lithium-Ion Batteries

Project ID: bat298

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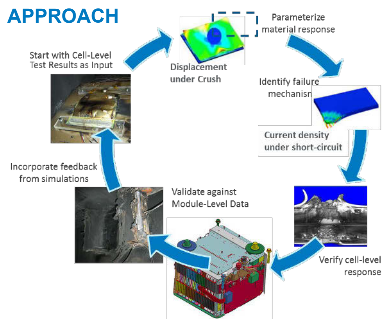
RELEVANCE

- DOE's Vehicle Technologies Office launched the Computer-Aided Engineering of Batteries (CAEBAT) project to develop validated modeling tools to accelerate development of batteries, in support of vehicle electrification R&D to reduce dependence on imported oil.
- This effort supports vehicle electrification R&D to produce plug-in electric vehicles (PEVs) that are as affordable, safe, and convenient as gasoline-powered vehicles for the American family.
- Over 45 different end users from the community have adapted the models approach developed under CAEBAT – of these 7 were new additions in 2018.
- Feedback from the first few sets of end-users has helped us identify priorities that will enable wider use of model-based design:
  - Expand identification of the model parameters (especially for mechanical properties) to high strain rates (up to 1000/s) and wider temperature window (as high as 180°C)
  - Increase computational efficiency by integrating both the mechanical and electrochemical models into a single platform (LS-DYNA)
  - Simulate complex failure modes including validation of the propagation models using multi-cell test cases
  - Close gaps between materials R&D and CAEBAT modeling tools

OBJECTIVES

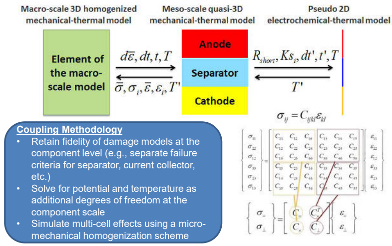
- Purpose: Assemble a multi-lab collaborative team, including experts from academia and industry, to make disruptive Computer Aided Engineering (CAE) design tools available for the battery community to:
  - Expedite path to $ 80/kWh electric vehicle (EV) battery costs by drastically reducing the number and duration of battery design cycles
  - Reduce module/pack costs by maximizing insight gathered on failure modes in batteries, from a limited subset of tests currently performed
- Our objectives for the March 2018-March 2019 period are to:
  - Integrate electrochemical simulations using user-defined elements in LS-DYNA to simultaneously solve electrochemical/thermal and mechanical models. This approach expedites cell-level simulations by up to 5 times.
  - Include complex loading conditions such as high strain-rates and shear-induced failure in mechanical-electrochemical-thermal (MECT) models
  - Develop materials database for mechanical properties abuse scenario
  - Present comparison of multi-cell propagation models

APPROACH



CAEBAT models simulate a variety of practical operating conditions and abuse response characteristics of batteries, tightly integrating material development and pack level performance. Virtual design using advanced computational tools significantly reduces development time and cost of batteries.

Mechanical-ECT Coupling Approach

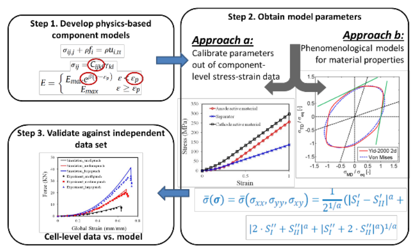


Coupling Methodology

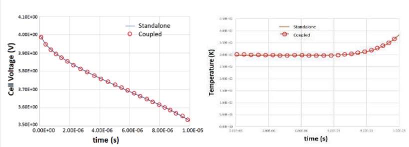
- Retain fidelity of damage models at the component level (e.g., separate failure criteria for separator, current collector, etc.)
- Solve for potential and temperature as additional degrees of freedom at the component scale
- Simulate multi-cell effects using a micro-mechanical homogenization scheme

In FY18, we implemented the above computational scheme using:
i) user-defined material models (loosely couple the electrochemical-thermal models with the mechanical response models)
ii) using custom user-defined elements that enable users to solve for concentration, potential and mechanical deformation in a tightly coupled simulation using LS-DYNA.

Constitutive Model Development Approach



Allowing the direct use of experimental datasets measured from components (electrode, current collector, separator, etc.) as input to cell-level simulations, or cell-level data as input to module level simulations, the approach provides alternatives to developing time-consuming material models, if the users choose to do so.

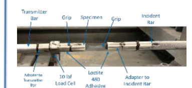


Six different case studies were developed to demonstrate scalability of the proposed approach to module and pack level simulations. These case files have been made available to the community.

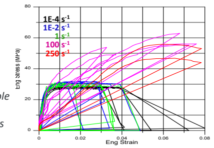
TECHNICAL ACCOMPLISHMENTS

Strain-rate Dependence and Dynamic Response

- In 2018, the team designed a test fixture to measure dynamic response of cell components at high strain rates (100-250 /s) in response to reviewers' comments from the previous AMR.
- The failure strains and yield strength of the electrodes are different at strain rates over 100/s, compared to the quasi steady-state response widely reported in the literature.
- These results are currently being into cell-level models.

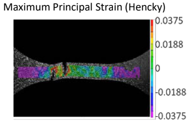


Dynamic test fixture design and sample results for strain-rate dependence of the mechanical response of electrodes



High-Speed Digital Image Correlation Data

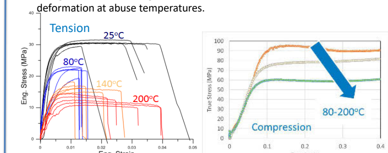
Maximum Principal Strain (Hencky)



In addition to the 1D stress-strain curves, high speed digital image correlation data (obtained at 200000 fps) showing complex fracture evolution patterns at high strain rates was also collected. We are pursuing 'Approach a' for implementing the constitutive models; development of phenomenological models for this complex data set is still very challenging.

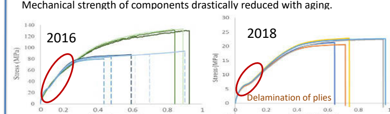
Mechanical Response at Abuse-Temperatures

- All component-level test data available thus far only included limited temperature effects.
- For the first time, in FY18, we collected stress-strain data at temperatures as high as 200oC, making the constitutive models relevant to simulate deformation at abuse temperatures.



Mechanical Response of Aged Cells

Cells were aged over an extensive period of 5 years and periodically disassembled to measure changes in failure parameters with aging.
Mechanical strength of components drastically reduced with aging.

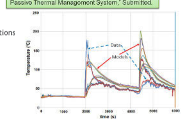


MULTI-CELL VALIDATION CASE STUDIES

- Four different sets of experimental data are currently being used towards multi-cell validation of the MECT models.

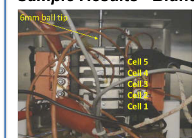
- *Case 1:*
  - 5 Ah LCO/Graphite chemistry cells
  - Pouch format cells
  - 5 cells stacked back-to-back with no electrical contact
  - Aluminum and Copper cooling plates of different thicknesses (1/8", 1/4", ½")
  - Compression from the top; cylinder indentation (bar crush) from the sides
- *Case 2:*
  - 6 Ah NMC/Graphite chemistry cells
  - Prismatic cells with aluminum cans
  - 5S1P (all cells electrically connected in series)
  - Blunt rod from the top and sides; different SOCs
  - Cells implanted with NREL's ISC device at different locations
- *Case 3:*
  - 32 Ah (LMO+Li-Nickel-Oxide)/Graphite chemistry cells
  - Laminate pouch cells
  - 2S2P electrical configuration
  - Bar crush following USABC protocol for modules
- *Case 4:*
  - 16 Ah (LMO+NMC/Graphite) chemistry cells
  - Pouch format cells
  - Modules of 45x5P w/ side and end brackets
  - Bar crush across two orientations

Q. Li, C. Yang, S. Santhanagopalan, K. Smith, J. Lamb, L.A. Steele, L. Torres-Castro, "Numerical Investigation of Thermal Runaway Mitigation in a Passive Thermal Management System," Submitted.

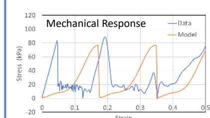


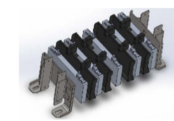
Y. Chen, S. Santhanagopalan, V. Babu, Y. Ding, "Dynamic Mechanical Behavior of Lithium-ion Pouch Cells Subjected to High-Velocity Impact", Composite Structures 2019, 218, 50-59

Sample Results - Blunt-rod Test Simulations

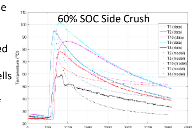


- 5S1P String of high-power 6 Ah Cells (NMC/Graphite)
- Module Voltage 17.75 V (60% SOC)
- Aluminum cooling plates
- Thermocouple locations (1-8) shown on schematic: TC2 recorded ambient temperature in the chamber
- Load cell capable of 50kN max. load
- EUCAR 2 response recorded for both top and side-crush

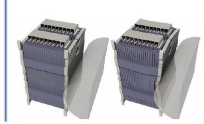




- For this dataset, the mechanical response was dominated by the properties of the prismatic cell can.
- The temperature response was controlled very well during the propagation simulations – the thermal mass of the cells contributed to the mitigation strategy.
- These models do not capture fracture of the case as a function of strain rate, or response under other complex loading conditions as yet.



Other Validation Studies Underway



- 4S5P modules tested in earlier phase
- Experimental data already available.
- module level mechanical-only simulations were completed under CAEBAT-II
- Coupling w/ ECT simulations currently being implemented using the simultaneous coupling approach outlined here.

MILESTONES

	Milestone Name/Description	Deadline	Milestone Type	Status
Computational Efficiency	M 1.2 Submit journal article investigating spatial heterogeneity due to electrode processing variations. Report on 3D microstructure electrochemical model algorithm enhancements for improved computational speed, accuracy, and scalability	12/31/2018	Qtr. Progress Measure	Complete
	M 1.2 Demonstrate electrochemical models enhanced with mechanical and/or multi-reaction mechanisms with application to VTO materials research	09/30/2019	Qtr. Progress Measure	On Track
Mechanical Abuse	M 2.1 Document implementation of mechanical abuse simultaneous coupling in the form of case studies (.k files) that can be distributed to end users	03/31/2019	Annual SMART Milestone	Complete+
	M 2.2 Present final report on the MECT models at the Vehicle Technologies Office Annual Merit Review	06/30/2019	Qtr. Progress Measure	On Track

FUTURE WORK

- In FY19, the team will complete validation studies for multi-cell test articles.
- We plan on making a databank of mechanical response for cell components at various strain rates and temperatures available. To the best of our knowledge, the high strain-rate data and high-temperature data presented in here is the most comprehensive characterization of mechanical properties of battery electrodes.
- We are planning a few more publications to include results from complex loading, high strain-rate results.
- Beyond 2020, with decommissioning of CAEBAT underway, we are working to integrate the modeling tools into various focused materials programs initiated by the DOE.

SUMMARY

Task 1. Computational Efficiency
- Efficiency and stability of mechanical models was significantly enhanced by implementing electrochemical models in LS-DYNA as User-Defined Elements.
- Six case studies were built and licensed out to participants from Industry for initial testing and their feedback is being incorporated into these tools.

Task 2. Simultaneously coupled mechanical-electrochemical-thermal model for mechanical abuse simulation
- Dynamic response of the cells was incorporated by measuring mechanical response of components at strain rates as high as 250 /s.
- Temperature range for property measurements was expanded (as high as 200°C) to account for property changes at high temperatures experienced by cell components under battery abuse.
- Multi-cell validation has been expanded to include four different sets of experimental data, with support from various partners.
- Complex failure modes and fracture response are currently being investigated. These are still very challenging, given the limited amount of prior work available in the literature.

Select Publications:

1. Y. Chen, S. Santhanagopalan, V. Babu, Y. Ding, "Dynamic Mechanical Behavior of Lithium-ion Pouch Cells Subjected to High-Velocity Impact", Composite Structures 2019, 218, 50-59.
2. X. Feng, C. Xu, S. Zheng, L. Wang, X. He, M. Ouyang, S. Santhanagopalan, "Investigating the thermal runaway mechanisms of lithium ion battery based on a comprehensive thermal analysis database", J. Electrochem. Soc. 2018 165(16): A3748-A3765.
3. S. Santhanagopalan, C. Yang, C. Zhang, "Effect of Aging on Mechanical, Electrochemical and Thermal Properties of Lithium Ion Cell Components", Presented at the IMLB 2018.

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