Development and Validation of a Simulation Tool to Predict the Combined Structural, Electrical, Electrochemical, and Thermal Responses of Automotive Batteries

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Ford Motor Company

2016 DOE Vehicle Technologies Office Annual Merit Review and Peer Evaluation Meeting
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Project ID: ES296

Acknowledgments

	Energy Storage R&A	Ted Miller Jim Marcicki, Xiao Guang Yang, Alex Bartlett, Valentina Mejia, Marty Ferman
	Passive Safety R&A	Saeed Barbat, James Cheng Yijung Chen, Omar Faruque, Min Zhu, Bill Stanko, Hongyi Xu
	Electrified Powertrain Engineering (EPE)	Chi Paik George Garfinkel, Amar Marpu
	Oak Ridge National Laboratory	Srdjan Simunovic, Sergiy Kalnaus, Srikanth Allu, John Turner, Abhishek Kumar
	Livermore Software Technology Corporation	Pierre L'Eplattenier, Inaki Caldichoury, Dilip Bhalsod

Overview

Timeline

- Start: January 1, 2016
- End: December 31, 2018
- Percent complete: 14%

Barriers Addressed

- Battery/Energy Storage R&D
  - Cost
  - Abuse Tolerance, Reliability and Ruggedness

Budget

- $4.375M total project funding
  - $3.5M DOE share
  - $875k Ford share
- No funding received in FY 2015
- Projected $750k DOE share for FY 2016

Subcontracts

- Project Lead: Ford Motor Company
- Subcontract: Oak Ridge National Laboratory (ORNL)

Relevance

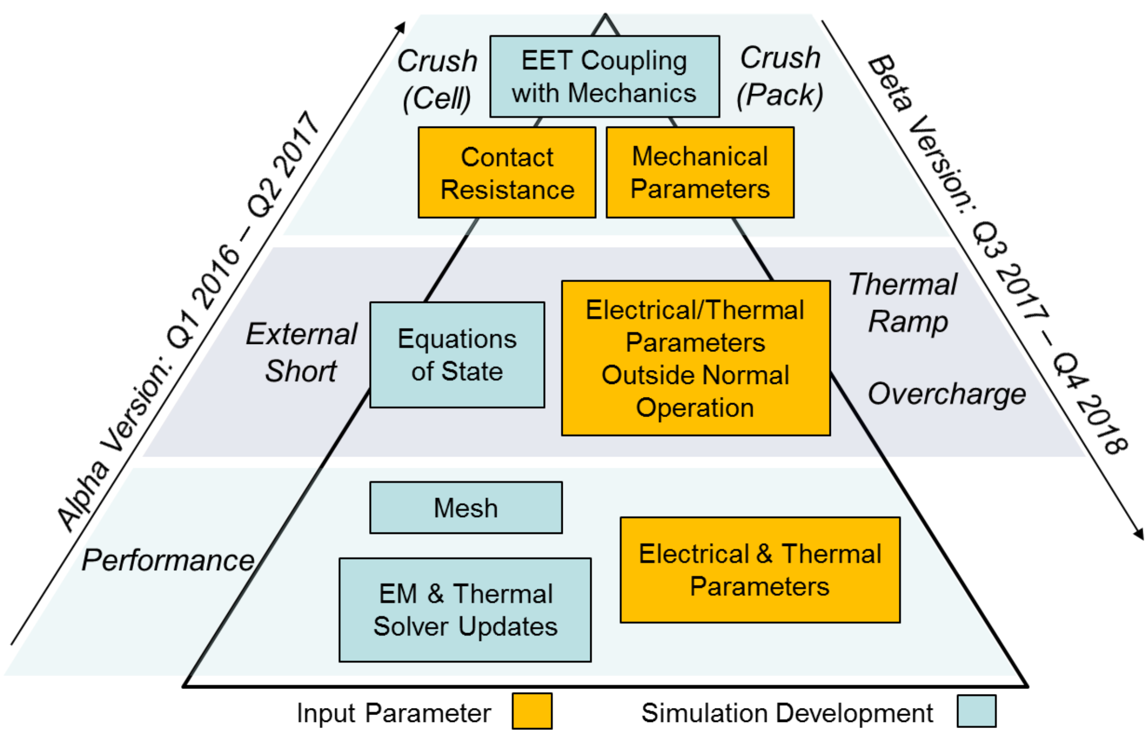
Overall project objective: Develop a practical simulation tool to predict the combined structural, electrical, electrochemical, and thermal (EET) responses of automotive batteries to crash-induced crush and short circuit, overcharge, and thermal ramp, and validate it for conditions relevant to automotive crash.

Barriers Addressed:

Cost ↓ by shortened development cycles and optimized crash protection systems

Abuse tolerance ↑ by delivering a predictive simulation tool to shorten or eliminate design-build-test prototype cycles and optimized crash protection systems

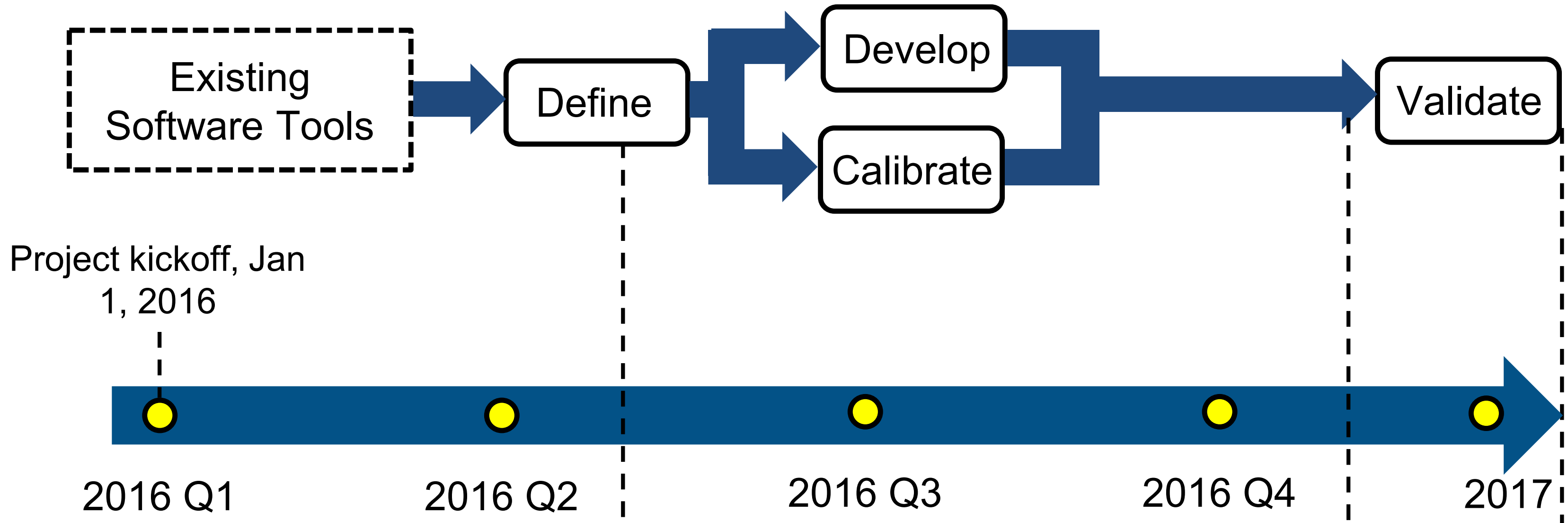
Project Plan



Tasks & Milestones for Budget Period 1

Tasks	2016 Q1	2016 Q2	2016 Q3	2016 Q4
Select and procure hardware for model validation	M1			
Formulate development assumptions for model		M2, M3		
Create multi-physics solvers and material models				
Identify and obtain required model inputs				
Integrate solvers into Alpha version model				DP1
Validation of Alpha version model			M4	

Approach/Strategy: Model Development



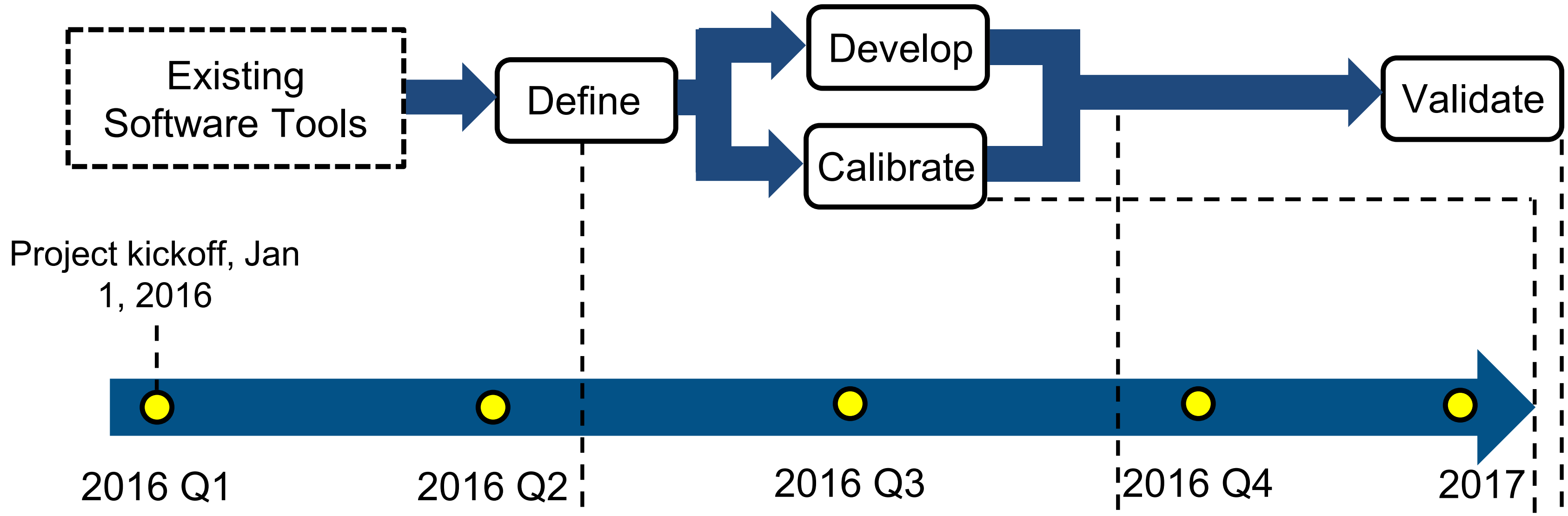
M2: Benchmarking analysis of existing models completed. Consider computational requirements, model robustness for typical case studies, and required inputs.
M3: Formulate development assumptions for solver enhancements. Target advancements that significantly reduce computational requirements and improve robustness beyond existing models.

DP1: Demonstrate preliminary version of CAE software for cell-level crush multi-physics response, prior to full-scale validation.

M6: Complete multi-physics solvers and material models.
M7: Integrate solvers into Alpha version model. Update user-interfaces for pre/post processing.

Not started | On-track | Complete

Approach/Strategy: Model Validation



M1: Select hardware for model validation activities. Choose cell formats and chemistries that are broadly applicable to the automotive market, with particular emphasis on high-energy cells.

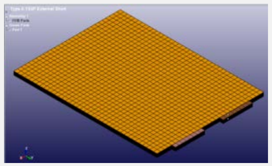
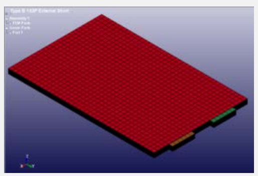
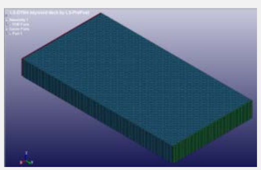
M4: Identify test site and define validation tests. Validation will primarily consist of high strain rate impact testing in a variety of orientations and energy levels.

DP2: Cell-level validation of simulation tool completed for full range of mechanical testing.

M5: Complete database of model inputs for model validation activities, including electrical, electrochemical, thermal, and mechanical inputs.

Not started | On-track | Complete

Technical Accomplishments and Progress: Hardware Selection

Mesh	Type	Cathode Chemistry and Format	Cell	Module	Pack
	A	NMC//LMO Blend Pouch	15 Ah 3.7 V 0.06 kWh	4P1S 5P4S	4S5P (x9) + 2S5P (x2)
	B	NMC Pouch	20 Ah 3.6 V 0.07 kWh	3P1S and 3P10S	
	C	LFP Prismatic	18 Ah 3.2 V 0.06 kWh	4P1S 5P2S	36S5P
To be developed	D	NMC Pouch	21 Ah 3.65 V	5P4S	4S5P (x9) + 2S5P (x2)
To be developed	E	Metal Oxide Blend Prismatic	60 Ah 3.65 V (est)	TBD	

Legacy Hardware ☐ Hardware sourced for this project ☐

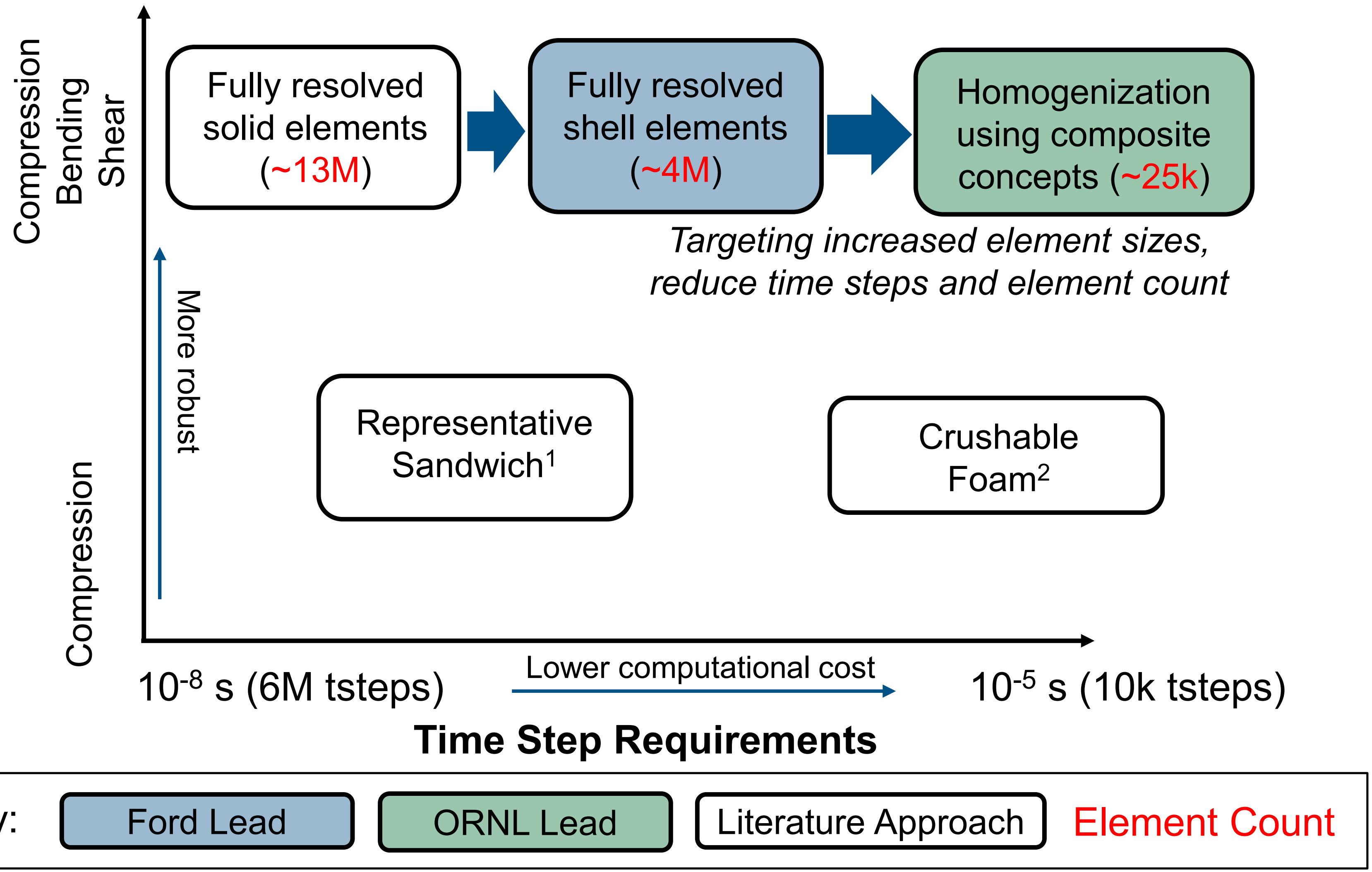
Legacy hardware supplemented with additional automotive-scale hardware for mechanically-focused validation

Technical Accomplishments and Progress: Model Development Assumptions

	Crash	Regulatory Crush	Overcharge/External Short/Thermal Ramp
Mechanics Time Scale	< 100 ms	> 10 s	> 10 s
EET Time Scale	ms to minutes		
Deformation Mode	Out-of-Plane or In-Plane Compression; Bending; Shear	Out-of-Plane Compression; In-Plane Compression	Internal Swelling; Separator Melting
Contact Locations	Unknown	Known	Unknown

3-D, transient finite element code needed to span these target applications
Methods to span time scales of mechanics and EET will be developed

Technical Accomplishments and Progress: Mechanical Model Benchmarking and Development Assumptions

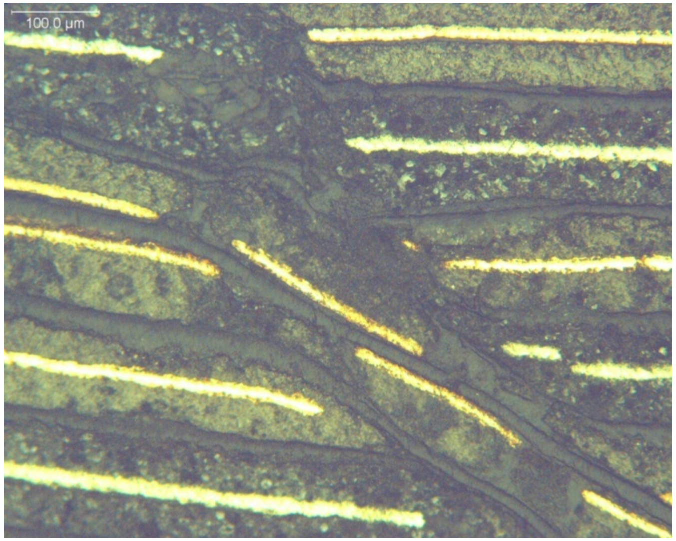


1) J. Power Sources, 290, 102 – 113 (2015). 2) J. Power Sources, 201, 307 – 321 (2012)

Technical Accomplishments and Progress: Mechanical Model Benchmarking and Development Assumptions

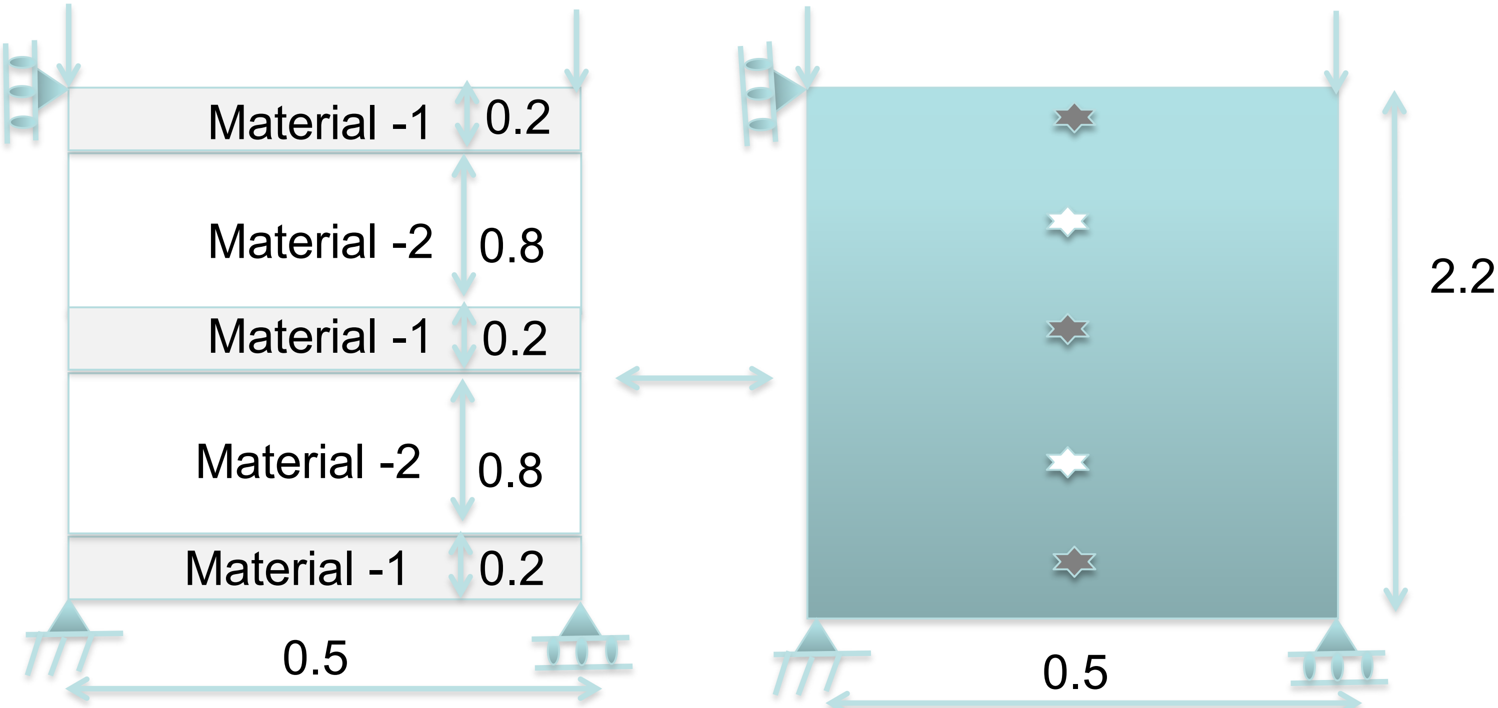
- Mechanical response is hierarchical (jellyroll to module)
- Jellyroll is a new material for impact modeling, its mechanical response under external load is not well understood
- Internal electrical short originates in the jellyroll
- Current models assume homogeneous displacements across battery components
  - Reasonable only for low deformation
- The onset and configuration of internal short depends on how the components deform and break

Technical Accomplishments and Progress: Mechanical Model Benchmarking and Development Assumptions



- Modeling deformation and the onset and configuration of short requires combination of new FEM element technology, constitutive models, interface, and failure models.
- Direct resolution of each layer in analysis is too computationally expensive.
- We are working with LSTC on the development of element formulations that will enable upscaling of internal kinematic and load transfer mechanisms of battery cells.

Technical Accomplishments and Progress: Mechanical Model Benchmarking and Development Assumptions

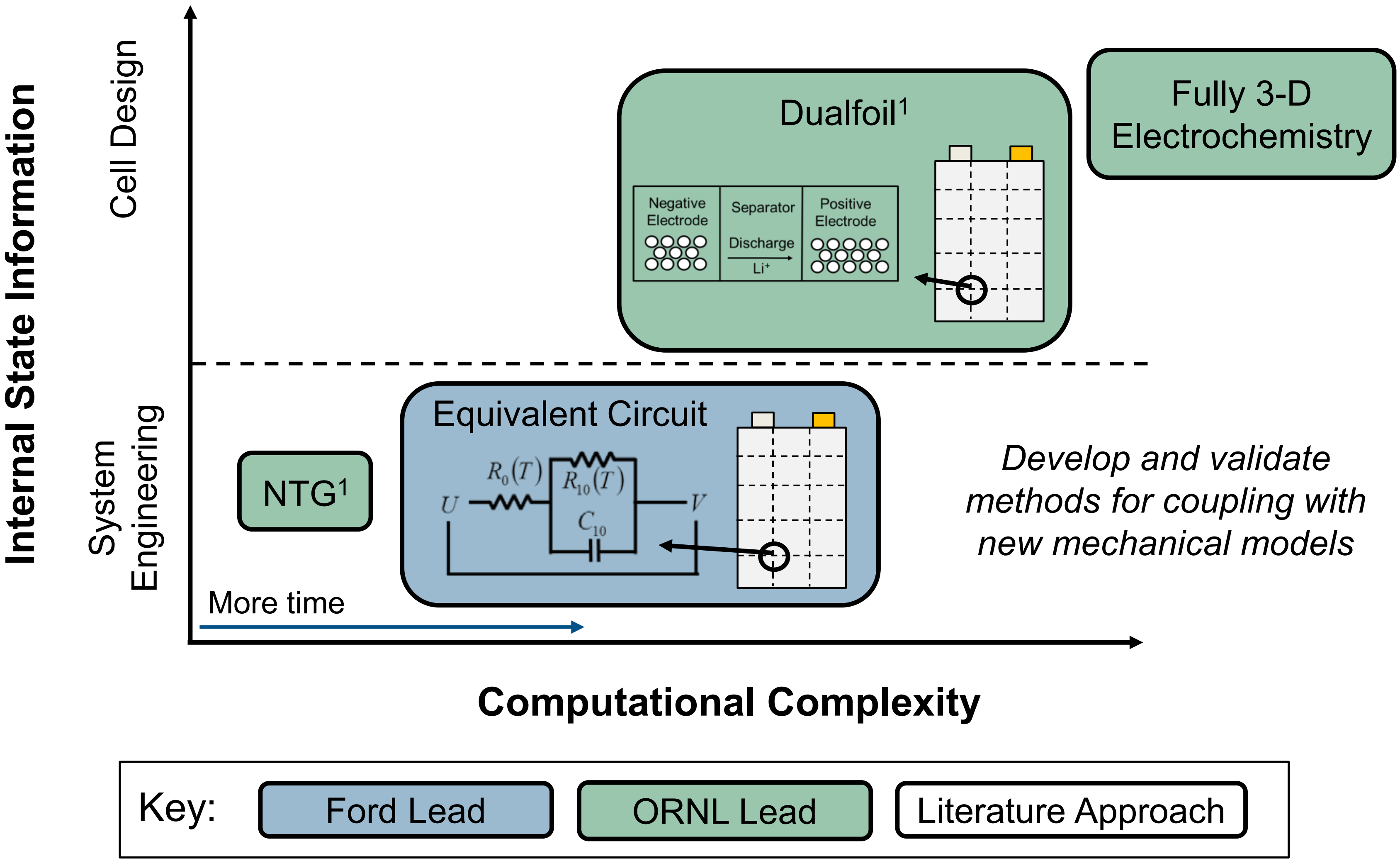


1 element for each material

Layered Solid

- Difference of the response between models that resolve every cell component and corresponding layered solids is used to determine limits of the current layered formulation and the new capabilities to develop and implement.

Technical Accomplishments and Progress: EET Model Benchmarking and Development Assumptions

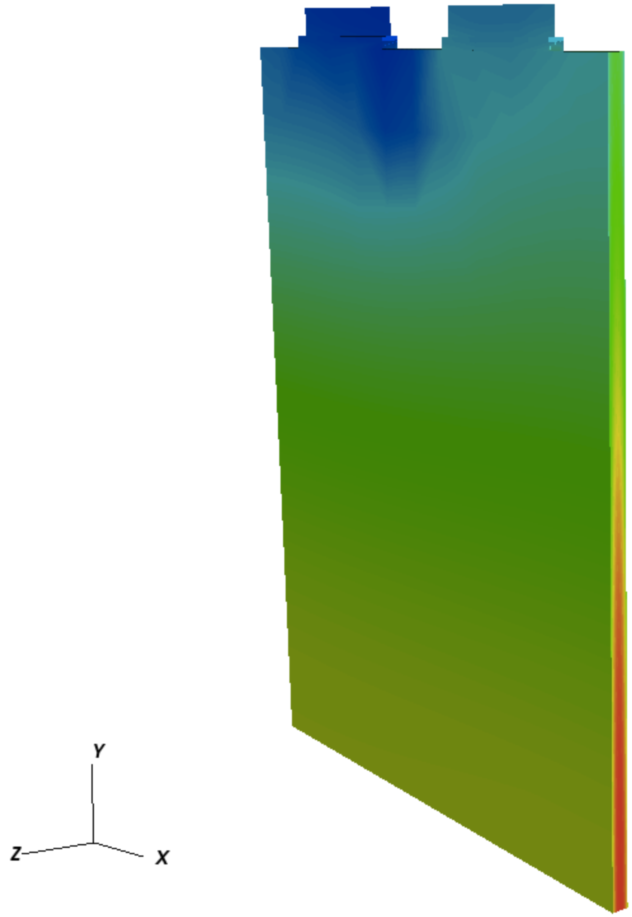


1) J. Power Sources, 246, 876 – 886 (2014).

Technical Accomplishments and Progress: EET Model Benchmarking and Development Assumptions

Properties from Literature*

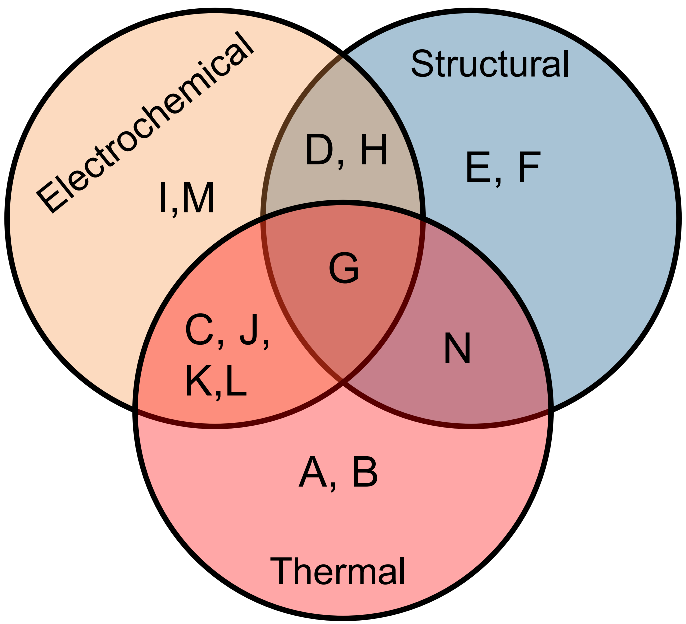
Symbol	Units	Anode (Carbon)	Separator	Cathode (NMC)
L	μm	54	10	58
ε_s	-	0.65	-	0.62
ε_e	-	0.33	0.48	0.29
ε_f	-	0.026	-	0.073
$c_s^{\max}$	mol/m^3	30813	-	51000
c_s^0	mol/m^3	20469	-	13872
c_e^0	mol/m^3		1300	
D_s	m^2/s	2.0x10^(-14)	-	7.5x10^(-10)
D_e	m^2/s		7.0x10^(-11)	
i_0	A/m^2	1.1	-	0.8
α_a	-	0.5	-	0.5
α_c	-	0.5	-	0.5
t_+^0	-		0.363	
σ	S/m	4.33	-	0.512
R_s	μm	6.35	-	5.15



*Chandrasekaran, Rajeswari. "Quantification of contributions to the cell overpotential during galvanostatic discharge of a lithium-ion cell." Journal of Power Sources 262 (2014): 501-513.

- Coupled 3D electrochemistry-thermal transport
- EC Boundary Conditions : Constant current discharge (1C)
- Peak temperature of 302 K

Technical Accomplishments and Progress: Identifying Model Inputs



Significant number of parameters are needed to populate the simulation inputs
Effort is underway to define and execute test methods for each input

Label	Property
A	Heat capacity
B	Thermal conductivity
C	System I-V response
D	Contact resistance
E	In-plane tensile F-D
F	Out-of-plane Compression F-D
G	Component dimensions
H	Component porosities
I	Active particle radii
J	Exchange current density
K	Electrical conductivity
L	Diffusion coefficient
M	Lithiation range of electrodes
N	Thermal expansion/shrinkage

Technical Accomplishments and Progress: Thermal Parameter Identification

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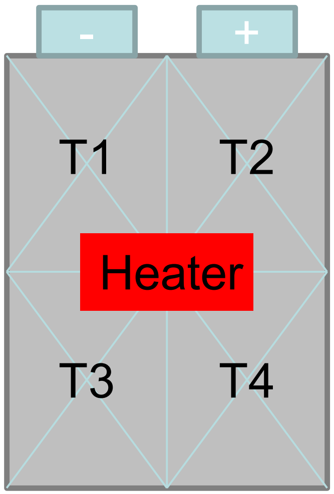
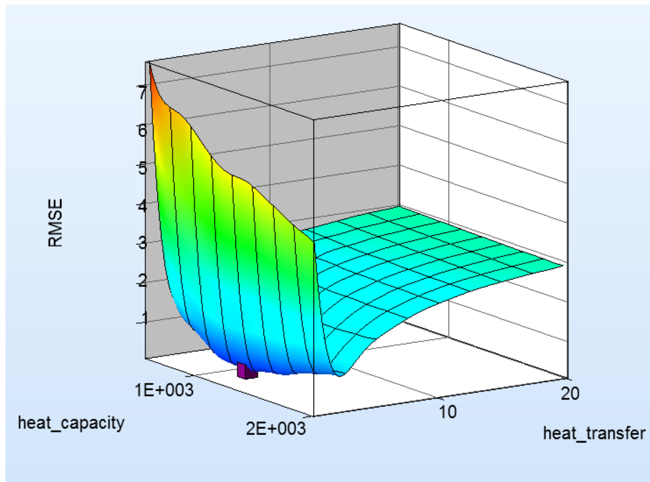
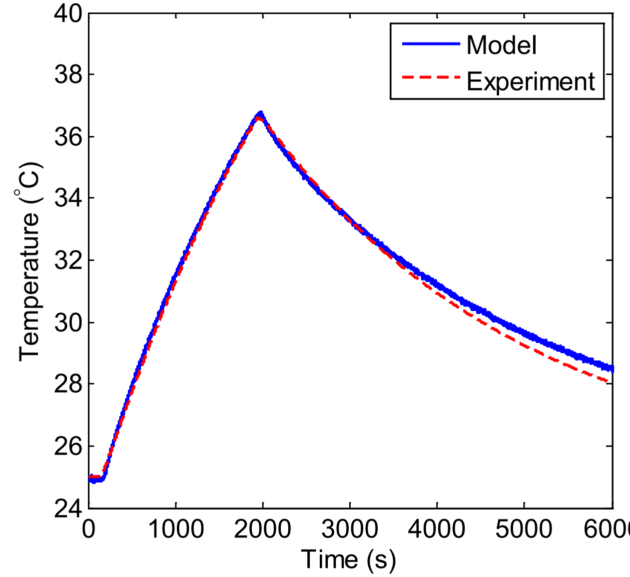
Heat Capacity Test Setup



Optimization Surface



Fitted Model and Experimental Temperatures at T1



Film heaters applied to known locations on cells; record heat delivered and thermal response

Minimize error of 3-D model using LS-OPT

Model-based optimization using quantified heat input determines cell thermal parameters

Technical Accomplishments and Progress: Mechanical Parameter Identification

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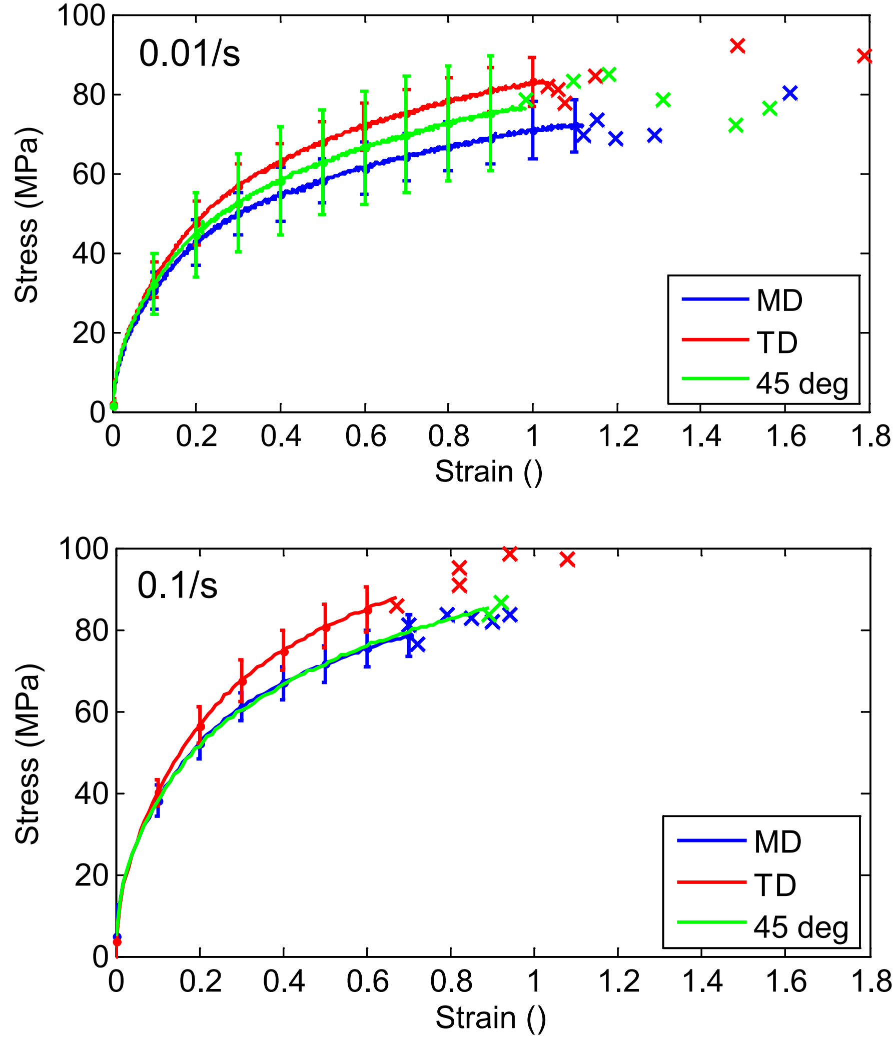
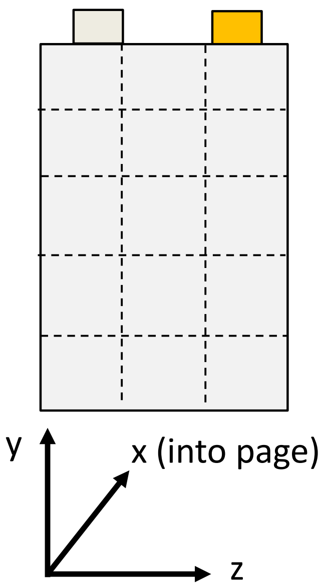
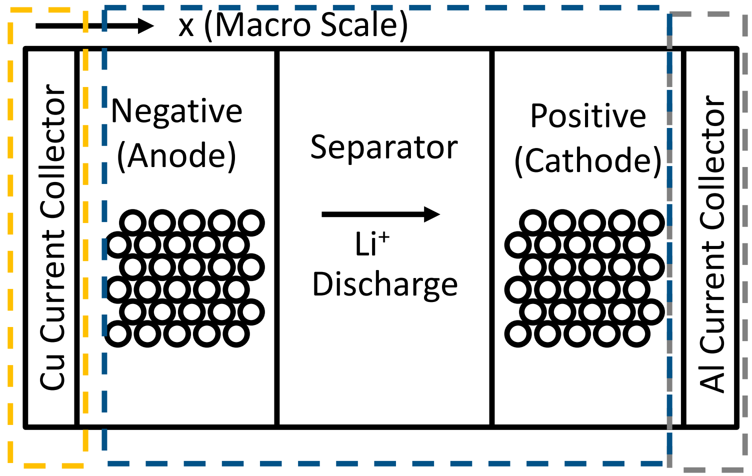
In-Plane Tensile Data – Type D Separator



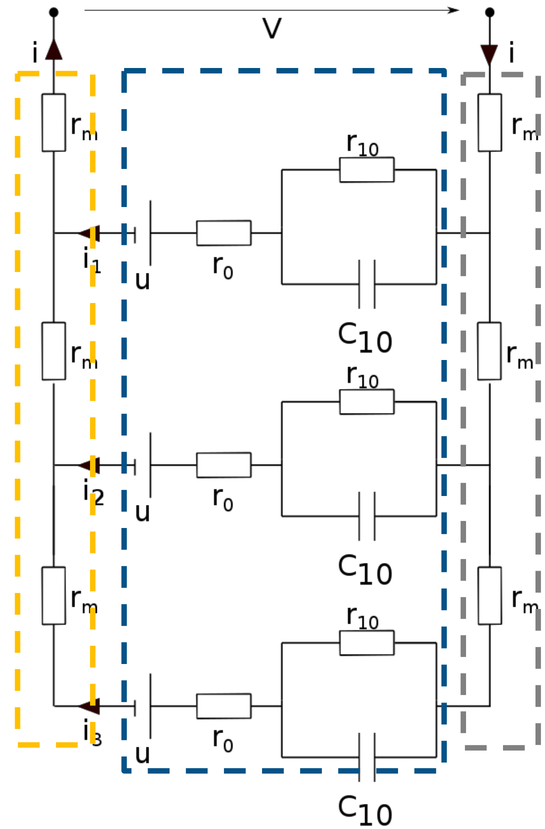
- In-plane tensile data for Type D cell separator shows minor strain rate dependence of energy absorption and strain to failure
- No orientation dependence within test repeatability
- Testing continues on other cell types and components
- Once mechanical data is fully compiled, constitutive models will be proposed

Technical Accomplishments and Progress: Creating Multi-Physics Solvers





- Current collectors transport electrons to/from tabs; modeled by resistive elements
- Jelly roll (anode – separator – cathode) transports Li+ ions; modeled with Randle circuit



r_0: Ohmic & kinetic

r_{10} & c_{10}: Diffusion

u: Equilibrium voltage (OCV)

r_m: Current collectors

Technical Accomplishments and Progress: Creating Multi-Physics Solvers

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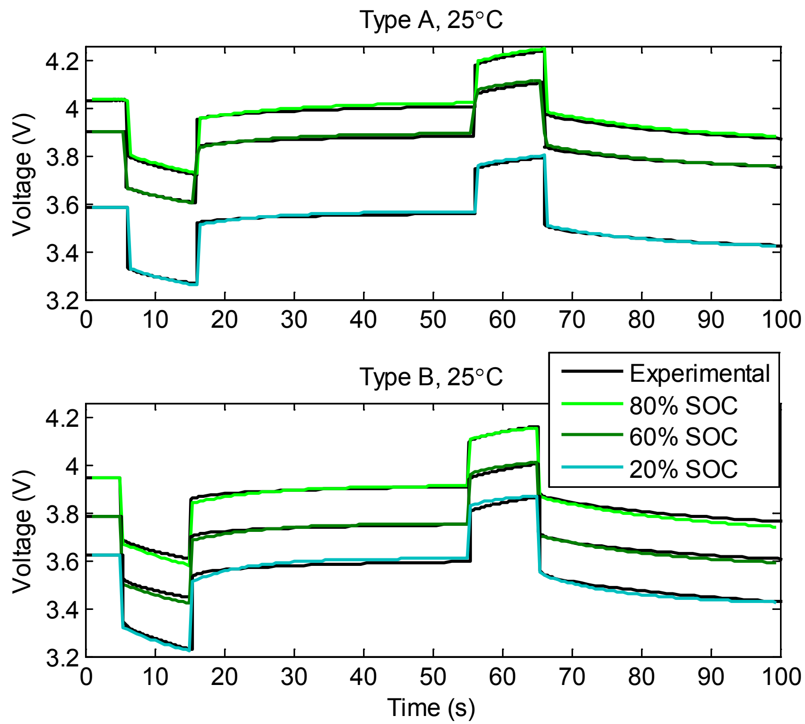

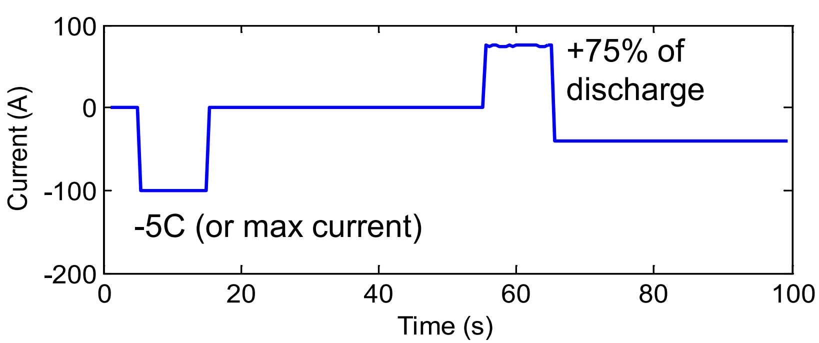

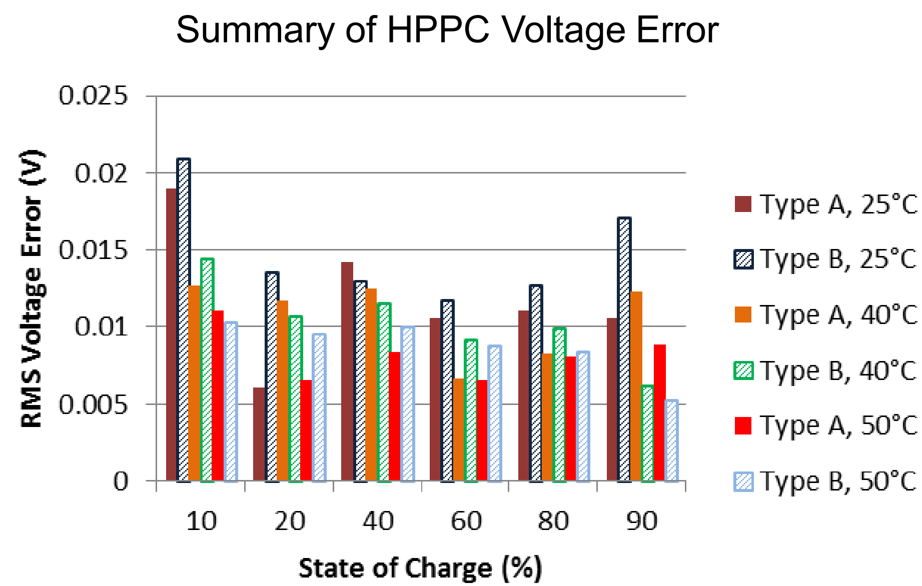

Short time voltage behavior captured well by model for both cell types

Technical Accomplishments and Progress: Creating Multi-Physics Solvers

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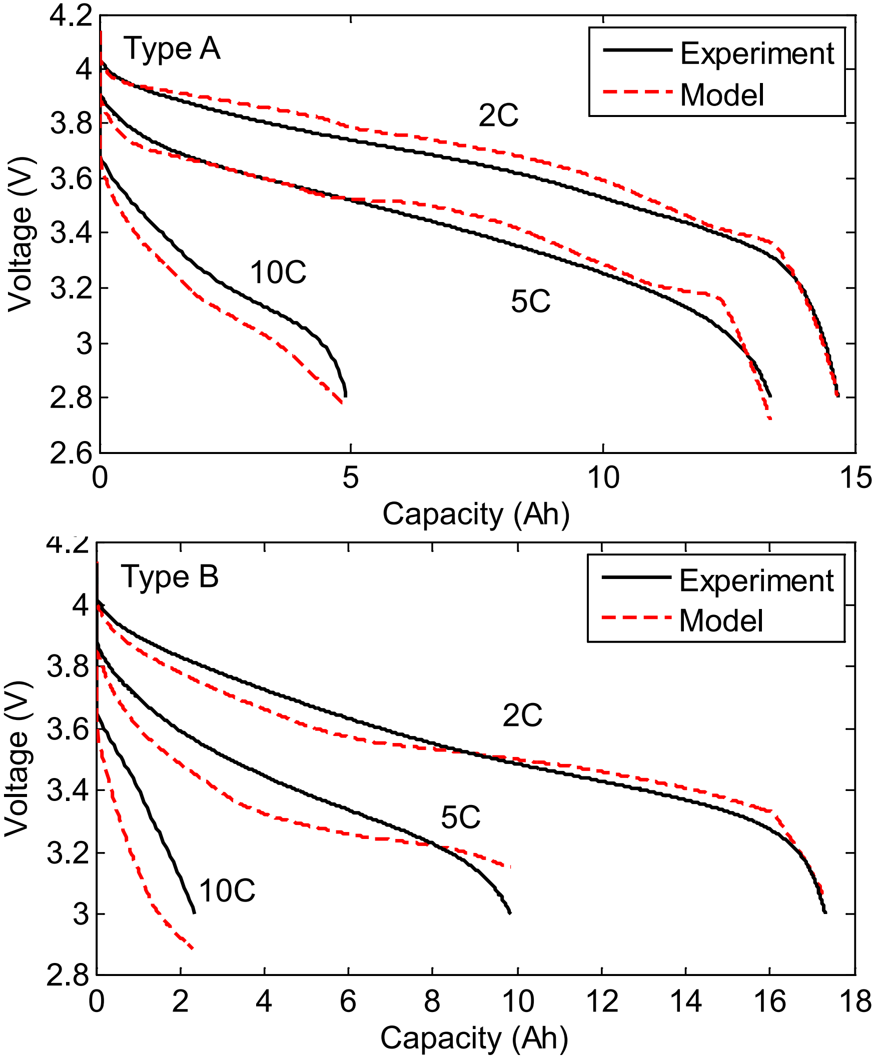
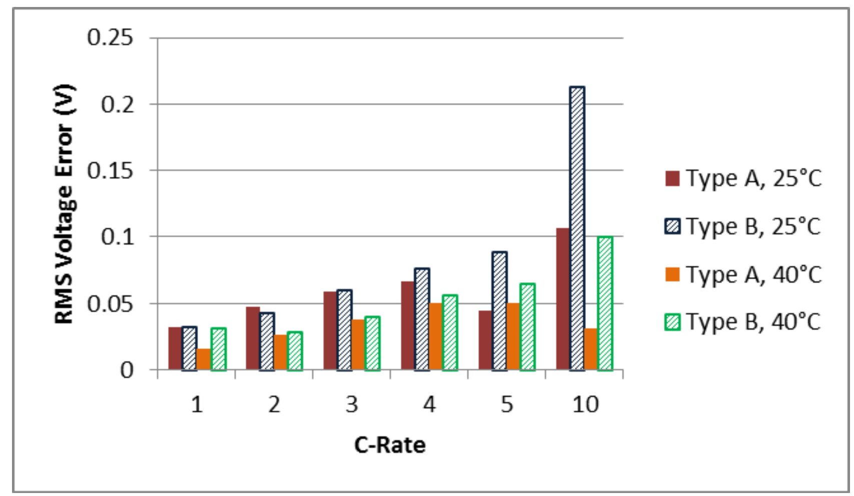
Model and Experimental Comparisons for Constant Current Discharge at Multiple Rates



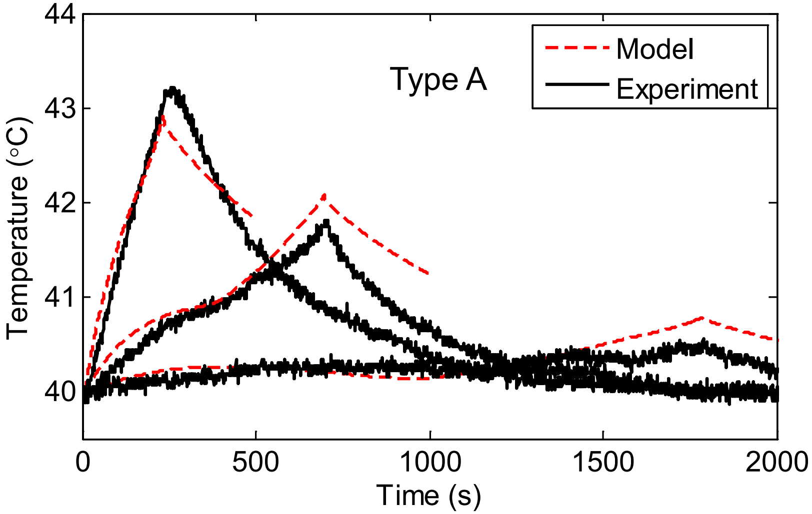
Summary of Constant Current Discharge Voltage Error

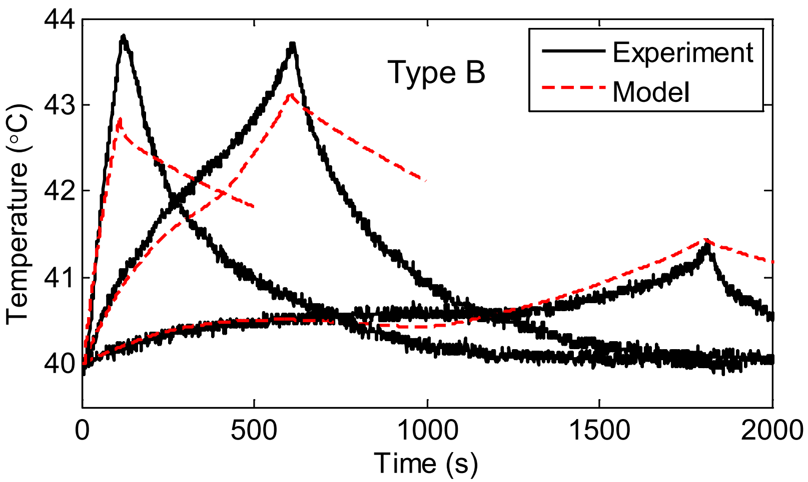


Longer time constant voltage behavior captured well by model at discharge rates up to 10C, particularly at high temperatures

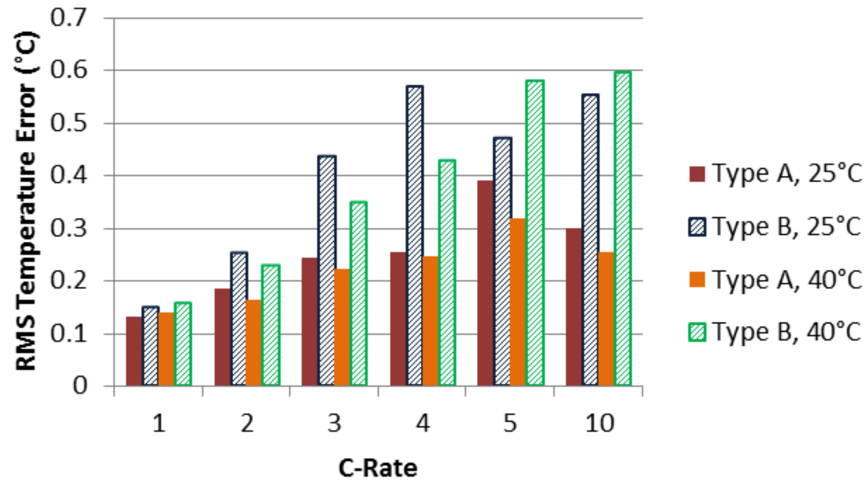
Technical Accomplishments and Progress: Creating Multi-Physics Solvers

Model and Experimental Comparisons for Constant Current Discharge at Multiple Rates





Summary of Constant Current Discharge Temperature Error



Thermal behavior of both cells captured well by model up to 10C

Response to Previous Year Reviewers' Comments

This is a new project that has not been reviewed previously

Collaboration and Coordination with Other Institutions

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Livermore Software Technology Corporation

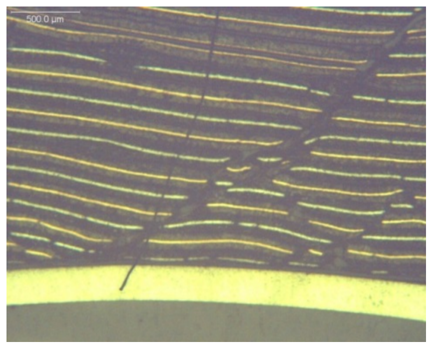
ORNL is developing methods to scale-up detailed mechanical and electrochemical simulations to reduce computational complexity while retaining high fidelity.

LS-DYNA® is the CAE software of choice for the project and contains key, battery-specific solver enhancements.

ORNL also collaborates with Lawrence Berkeley National Laboratory and Sandia National Laboratory under ES295

Remaining Challenges and Barriers

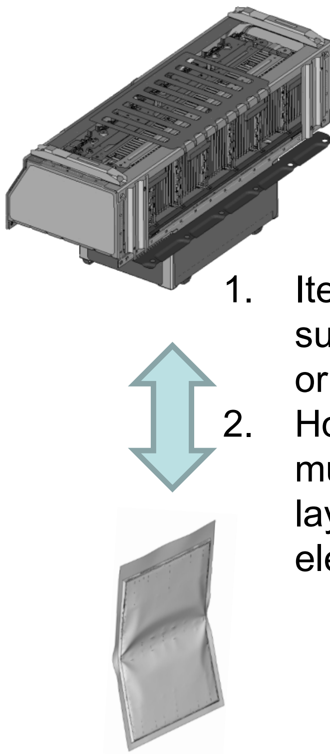
Improve Understanding of Criteria for Defining Mechanical Failure and Onset of Internal Short Circuits



1. Iterative methods such as sub-cycling, sub-modeling, or adaptive re-meshing
2. Homogenization of mutliple, thin, component layers into thicker elements

J. Power Sources, 306, 424-430, (2016)

Develop methods to span length scales involved in cells, modules, and packs with reasonable computational cost

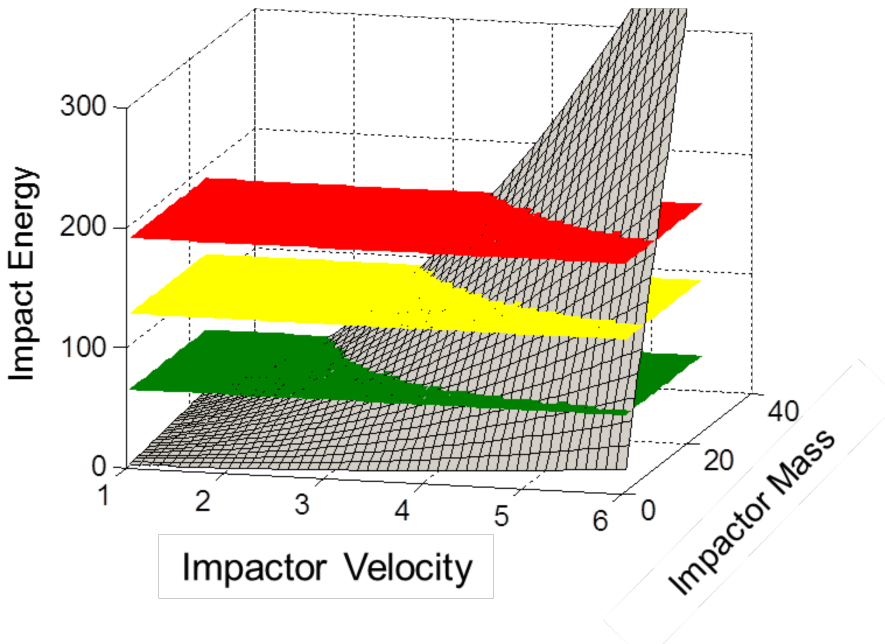


1. Iterative methods such as sub-cycling, sub-modeling, or adaptive re-meshing
2. Homogenization of mutliple, thin, component layers into thicker elements

Proposed Future Work

- **Near-Term**
  - Complete development assumptions for model
  - Begin integration of solvers for multi-physics predictions in abuse scenarios
  - Select test site and define validation tests
  - Continue to identify and execute cell characterization experiments

- **Mid-Term**
  - Complete input database for project hardware
  - Conduct validation experiments at multiple impact energy levels
  - Validate Alpha version of model for cell-level abuse testing
  - Document development assumptions for Beta version



- **Long-Term**
  - Conduct additional characterization experiments for Beta version input database
  - Perform solver enhancements for Beta version model
  - Validate Beta version of model for module- and pack-level impact testing

Summary

- **Relevance**
  - Develop and validate a simulation tool for battery abuse scenarios, including crash-induced crush, short circuit, overcharge, and thermal ramp
  - Target accelerated development of more abuse tolerant energy storage systems, and reduce cost by shortening prototype cycles
- **Approach/Strategy**
  - Define model requirements, then document model inputs in parallel with solver enhancements
  - Conduct validation testing for multiple hardware formats, chemistries, and scales, while leveraging historical data
- **Technical Accomplishments and Progress**
  - Equivalent circuit models with spatial and thermal dependence have been implemented in LS-DYNA, and validated for large-format pouch cells
  - Parameterization methods to obtain inputs governing the electrical, thermal, and mechanical response during abuse are under development
- **Collaborations and Coordination with Other Institutions**
  - Key computational methodologies from ORNL
  - LS-DYNA is the CAE software of choice
- **Proposed Future Work**
  - Define and execute validation tests at the cell level (year 1 and 2) and module to pack levels (year 2 and 3)
  - Deepen understanding of mechanical failure criteria for linking mechanics with the onset of short circuits

Technical Back-Up Slides

Gantt Chart

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			BP 1				BP 2				BP3			
DOE Task	DOE Task	Description	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 5	Qtr 6	Qtr 7	Qtr 8	Qtr 9	Qtr 10	Qtr 11	Qtr 12
0	Task 0.0	Project Management and Planning												
	Task 0.1	Kick-Off meeting												
	Task 0.2	Collaboration with National Laboratory												
1	**Task 1**	**Develop Alpha Model**												
	Task 1.1	Formulate Development Assumptions for the Model			M2 & M3									
	Task 1.2	Select and Procure Hardware for Use in Model Validation		M1										
	Task 1.3	Create Multi-Physics Solvers and Material Models					DP1							
	Task 1.4	Identify and Obtain Required Model Inputs												
	Task 1.5	Integrate Solvers into Alpha Version Model												
	Task 1.6	Validation of Alpha Version Model												
	1.6.1	Identify Test Site and Define Validation Tests				M4								
	1.6.2	Execute Tests and Compile Data												
	1.6.3	Comparative Analysis of Model and Experiments												
2	**Task 2**	**Complete Alpha Model & Begin Beta Model**												
	Task 2.1 (1.3)	Create Multi-Physics Solvers and Material Models						M5						
	Task 2.2 (1.4)	Identify and obtain required model inputs							M6					
	Task 2.3 (1.5)	Integrate Solvers into Alpha Version Model							M7					
	Task 2.4 (1.6)	Validation of Alpha Version Model									DP2			
	2.4.1 (1.6.2)	Execute Tests and Compile Data												
	2.4.2 (1.6.3)	Comparative Analysis of Model and Experiments												
	Task 2.5	Formulate Development Assumptions for the Beta Model								M8				
	Task 2.6	Select and Build Hardware for use in Beta Model Validation												
	Task 2.7	Create Multi-Physics Solvers and Materials Models for Beta Version												
3	**Task 3**	**Complete Beta Model**												
	Task 3.1 (2.6)	Select and Build Hardware for use in Beta Model Validation										M9		
	Task 3.2 (2.7)	Create Multi-Physics Solvers and Material Models for Beta Version											M10	
	Task 3.3	Identify and Obtain Required Model Inputs for Beta Version											M11	
	Task 3.4	Integrate Solvers into Beta Version Model												
	Task 3.5	Validation of Beta Version Model												
	3.5.1	Identify Test Site and Define Validation Tests												
	3.5.2	Execute Tests and Compile Data												
	3.5.3	Comparative Analysis of Model and Experiments												M12
		△ Milestone												
		☆ Go/No-Go Decision Point												

Milestone and Go/No-Go Definitions

Budget Period	Task	Description	Type	Start Date	End Date
BP1	1.2	Hardware selected	M1	1/1/2016	3/31/2016
	1.1	Analysis of existing models completed	M2	1/1/2016	6/30/2016
	1.2	Assumptions formulated	M3	1/1/2016	6/30/2016
	1.6.3	Test site selected	M4	6/1/2016	9/30/2016
	1.5	Preliminary version of software demonstrated	DP1		12/31/2016
BP2	1.4/2.2	Cell characterization experiments complete	M5	4/1/2016	3/31/2017
	1.5	Multi-physics solvers complete	M6	4/1/2016	6/30/2017
	1.5/2.3	Model integration complete	M7	10/1/2016	6/30/2017
	2.5	Beta model development assumptions	M8	7/1/2017	9/30/2017
	2.4/1.6	Alpha version completion	DP2		12/31/2017
BP3	3.1	Select & build hardware complete	M9	7/1/2017	3/31/2018
	3.1	Beta model validation complete	M10	1/1/2018	9/30/2018
	2.7/3.2	Multi-physics solvers complete	M11	1/1/2018	6/30/2018
	3.5.3	Comparative analysis of model and experiments	M12	10/1/2018	12/31/2018