Integrated Multiphysics Modeling for Improving Li-Ion Battery Pack Safety

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NREL Battery Modeling Capabilities

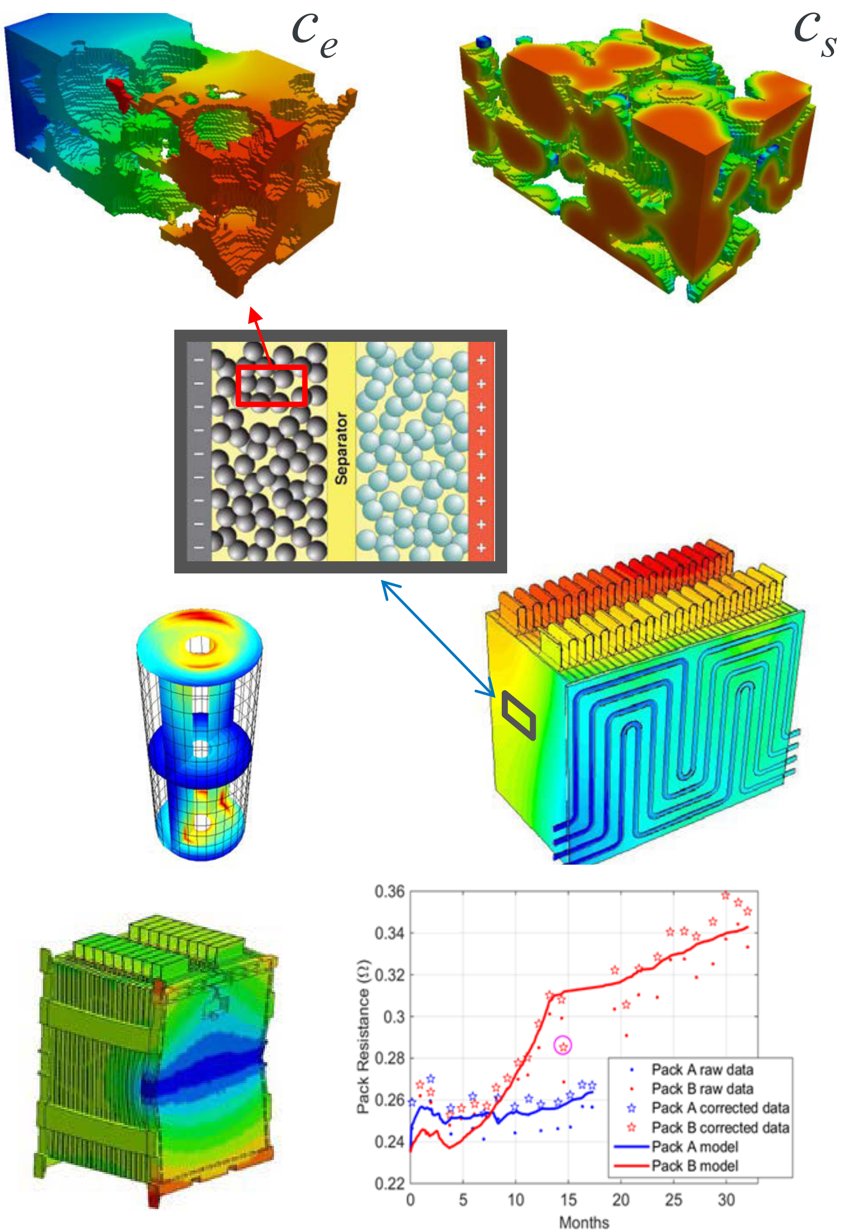
- **Microstructure**
  - Tomography
  - Homogenization, analysis
  - 3D echem simulation
  - Stochastic reconstruction

- **Macro-homogeneous modeling**
  - Dual electrode
  - Half cell
  - Electrochemical parameter ID

- **MSMD 3D cell & pack level**
  - Thermal/electrical design

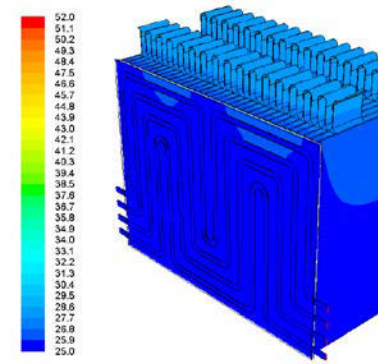
- **Safety**
  - Thermal runaway (TR)
  - Internal short circuit (ISC)
  - Mechanical abuse

- **Life**
  - Physics-based surrogate models
  - System design and real-time control

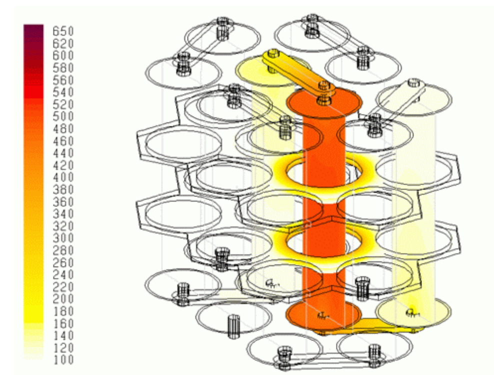


Integrated Multiphysics Modeling for Li-Ion Battery Safety Engineering

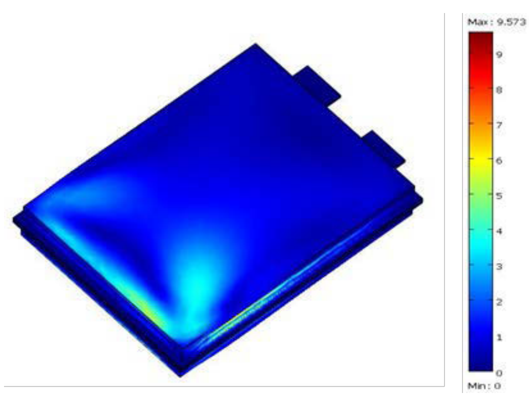
- Battery CAE tools are effective in evaluating battery safety design
  - Insightful understanding of failure thresholds
  - Failure propagation mechanism for each component within a unit
  - Better explanation of test data results in testing recommendations
  - Reducing design cycles and expense, and accelerating battery production development.



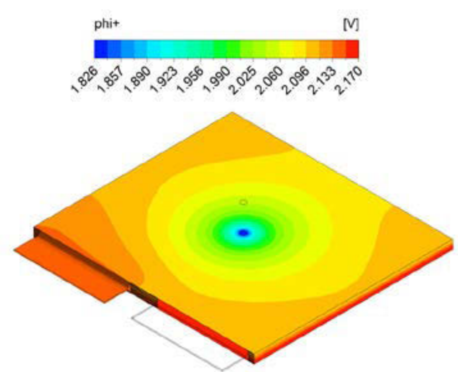
TMS



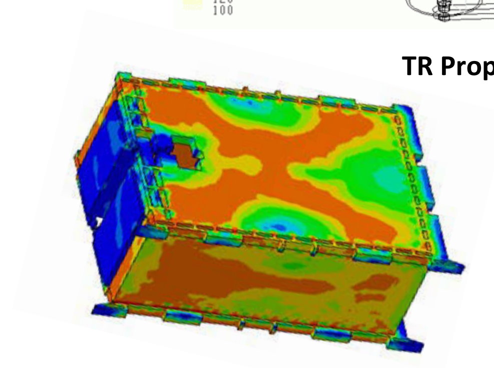
TR Propagation



Swelling of a Pouch Cell During a Hot-Box Test

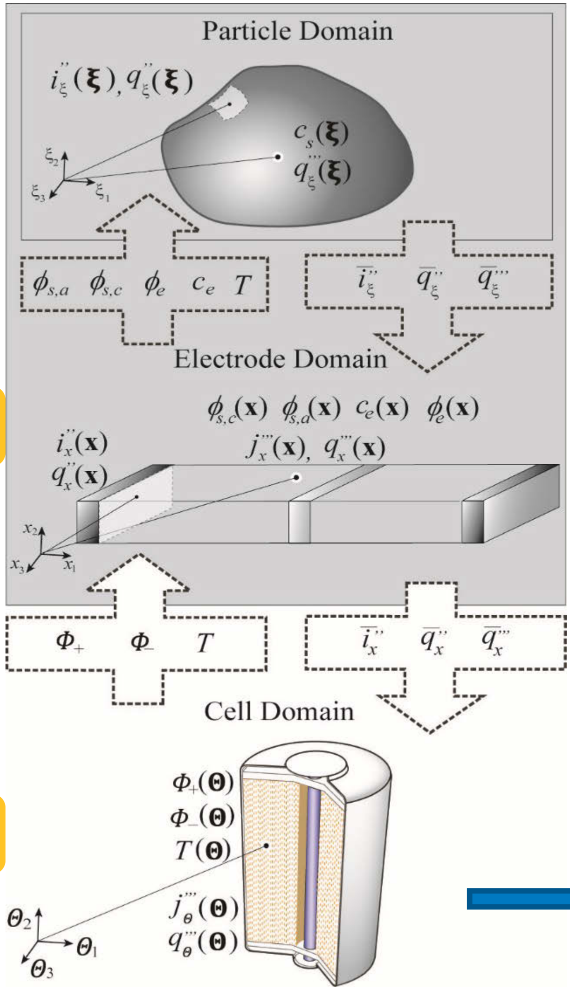


Potential under ISC



von Mises Stress Contours for Side Vs Edge Impact on Module

Integrated MSMD-Safety Strategy



EDM

CDM

NREL EDM Library

EDM- Electrochemical : NTGK

EDM- Internal Short Circuit (ISC)

EDM- Abuse Reaction Kinetics

Linking Protocol

- NREL EDM – Fluent API

CDM

- SPPC CDM-electrothermal model in ANSYS® Fluent® MSMD-module

Investigation of Thermal Runaway Tests

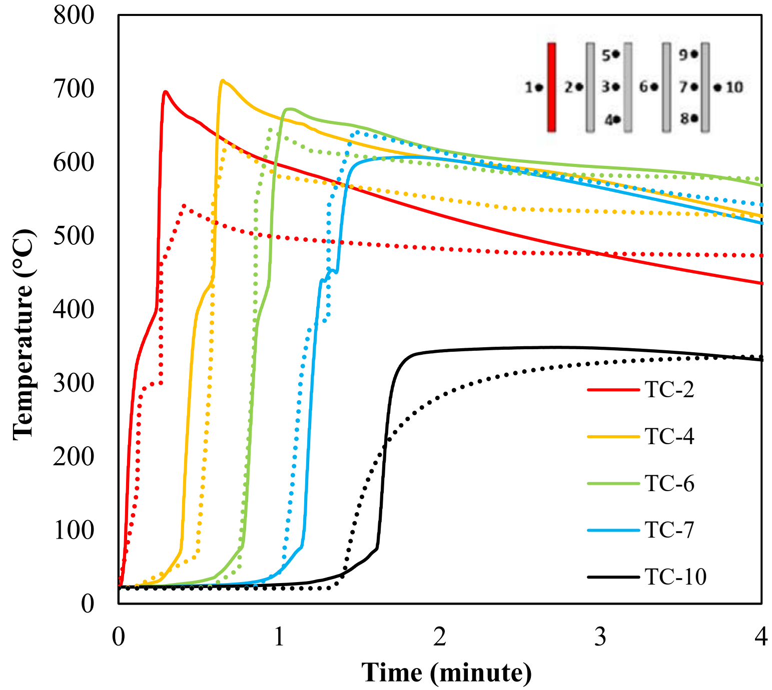
- 3Ah LCO Pouch Cell with an initial SoC 100%
- 5 Cells packed closely without electrical connection
- Trigger cell is a edge cell, failure initiated by a mechanical nail penetration along width axis of edge cell within 1.25 second

Tests done by BATlab in Sandia National Laboratories

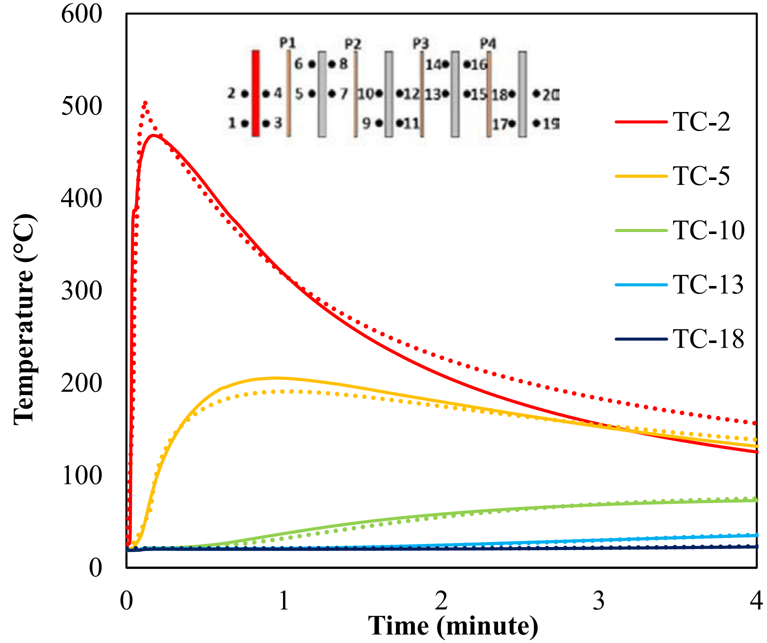
Case	Passive Thermal Management
Baseline	No thermal management
A1	3.2 mm Al plates
A2	1.6 mm Al plates
A3	0.8 mm Al plates

Effect of Heat Sink on TR Propagation

Baseline, no mitigation



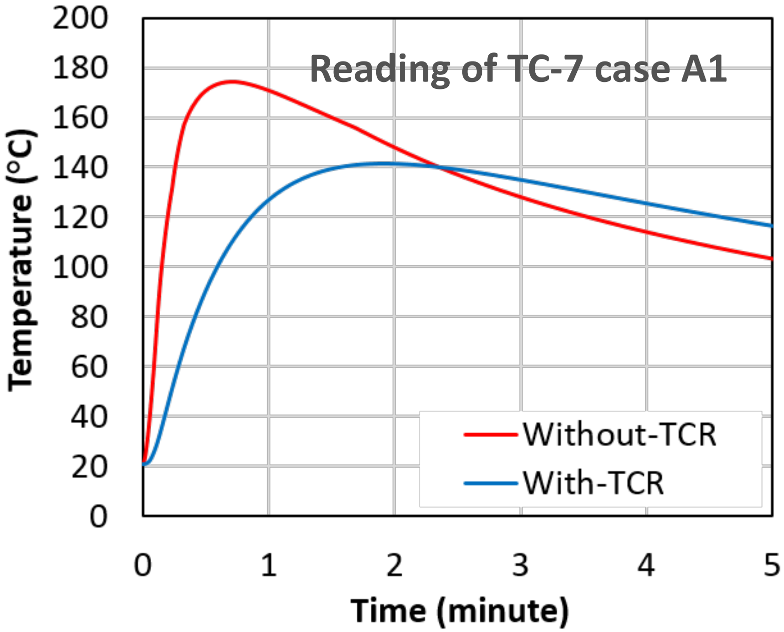
A1, successful mitigation



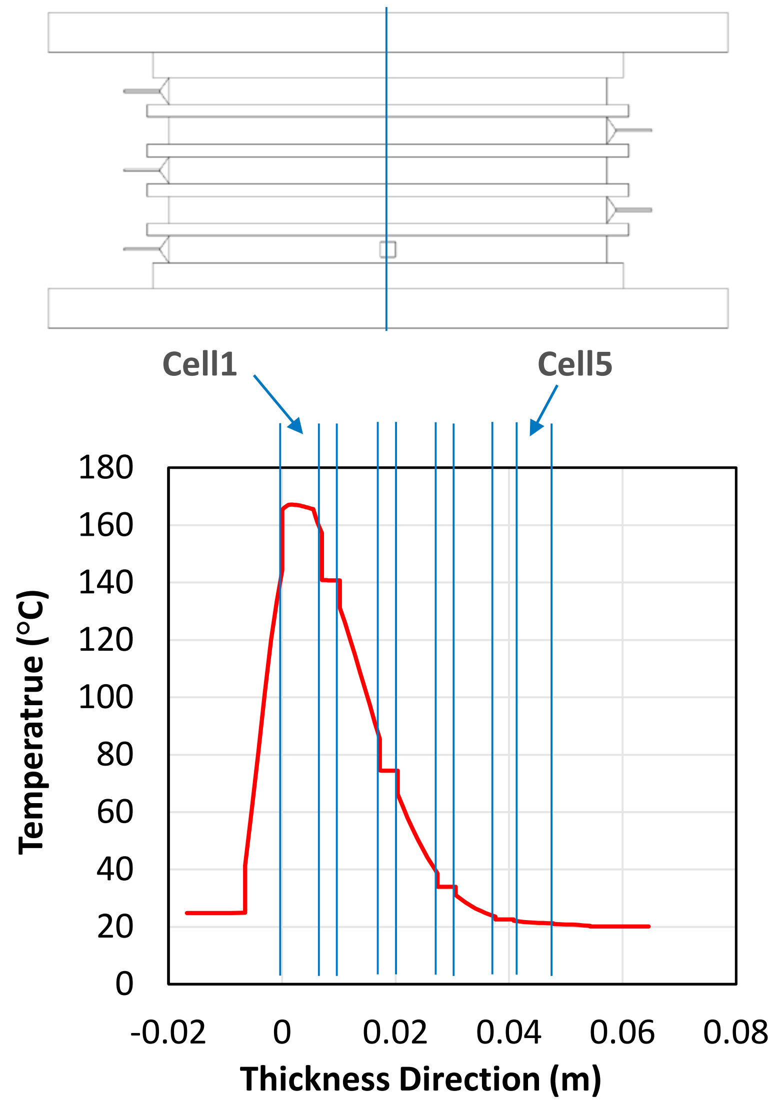
- Model validated again testing results for successful and non-successful cases
- Thermal mass is vital for passive control of thermal runaway.

$$\int_{t1}^{t2} q dt = (mC_p\Delta T)_{trigger\ cell} + \boxed{(mC_p\Delta T)_{Al\ plate}} + (mC_p\Delta T)_{neighbor\ cell} + \sum_{others} (mC_p\Delta T)_{others}$$

Effect of Thermal Contact Resistance (TCR)



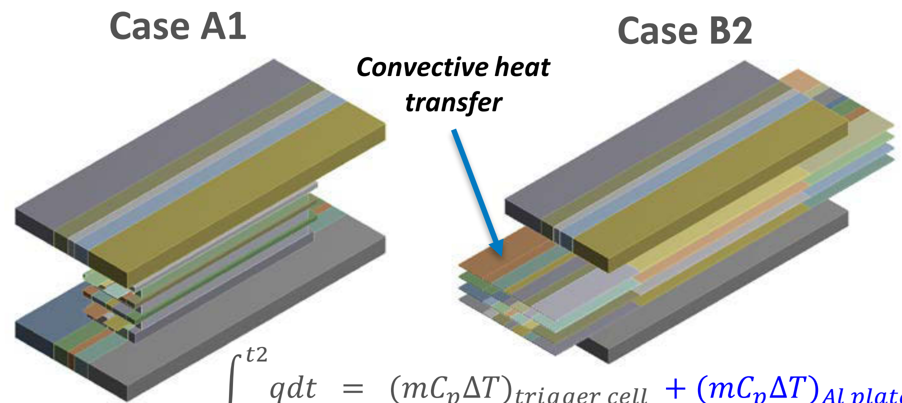
Temperature Distribution along Center Line



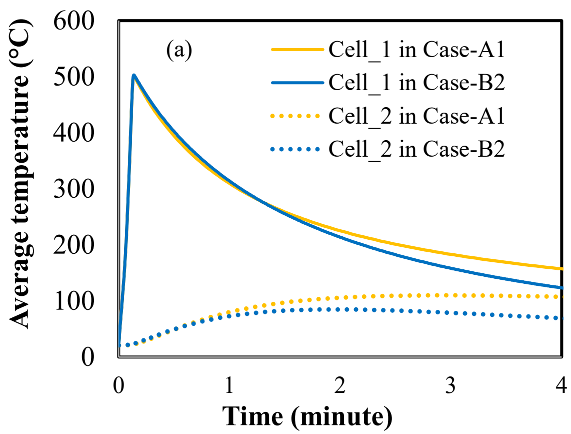
- Thermal contact resistance between cell and heat sink cannot be neglected in the 3D simulation of thermal runaway propagation
- It is valuable in reducing the severity of thermal shock.

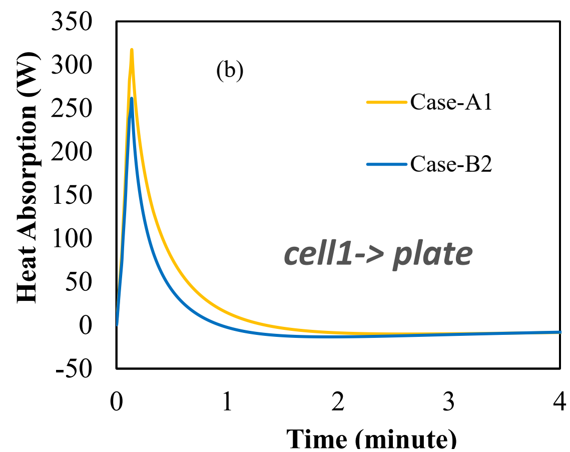
Geometric Shape Study

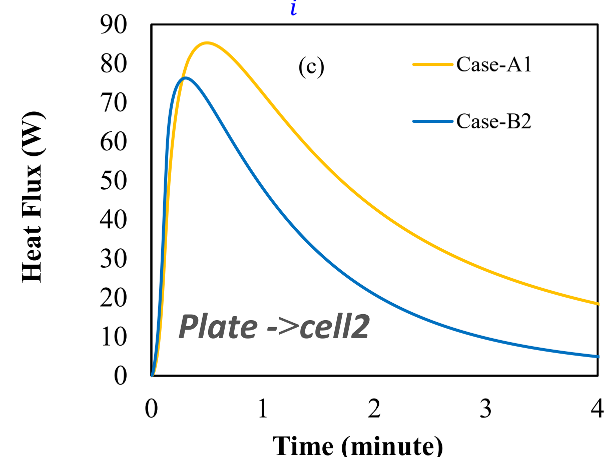
Case No.	A1	B2
Thickness	3.2mm	0.8
Surface Area	**0.005054 m²**	**0.020216 m2**
Thermal Mass Ratio	0.64	0.64



$$\int_{t1}^{t2} q dt = (mC_p\Delta T)_{trigger\ cell} + (mC_p\Delta T)_{Al\ plate} + (mC_p\Delta T)_{neighbor\ cell} + \sum_i (mC_p\Delta T)_i$$



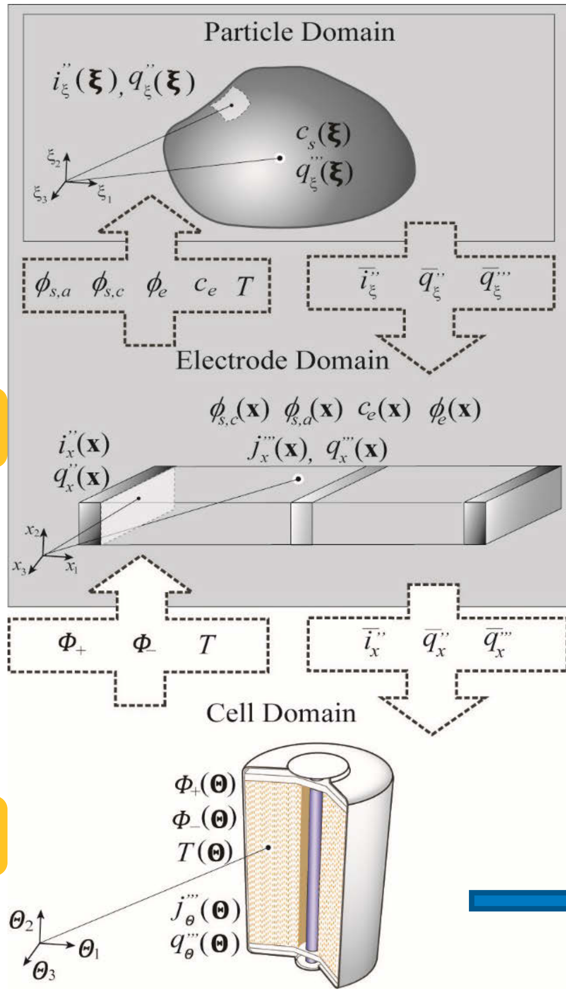




- Case A1 and B2 both mitigate thermal runaway propagation successfully
- Aluminum fin can be geometrically optimized to enhance heat dissipation out of the system.

Integrated MSMD-Safety Strategy

EDM



CDM

NREL EDM Library

- EDM- Electrochemical : NTGK
- EDM- Internal Short Circuit (ISC)
- EDM- Abuse Reaction Kinetics
- **EDM- Gas Kinetics**

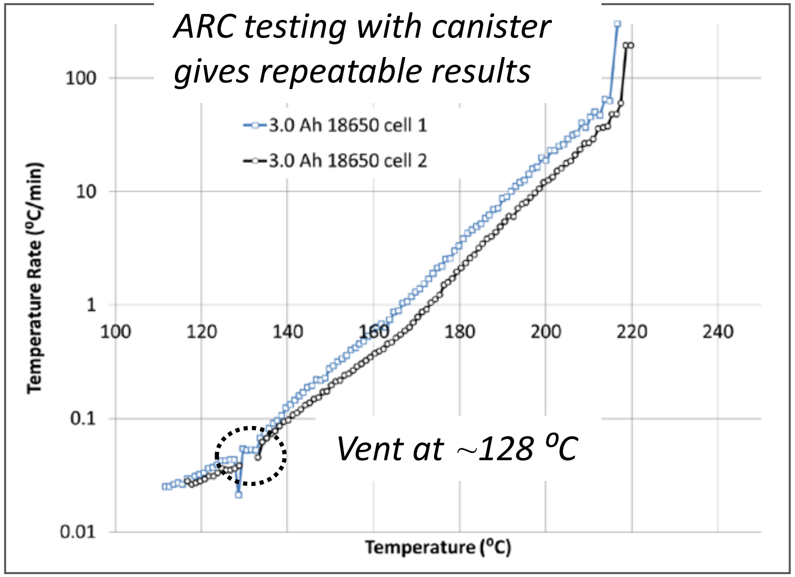
Linking Protocol

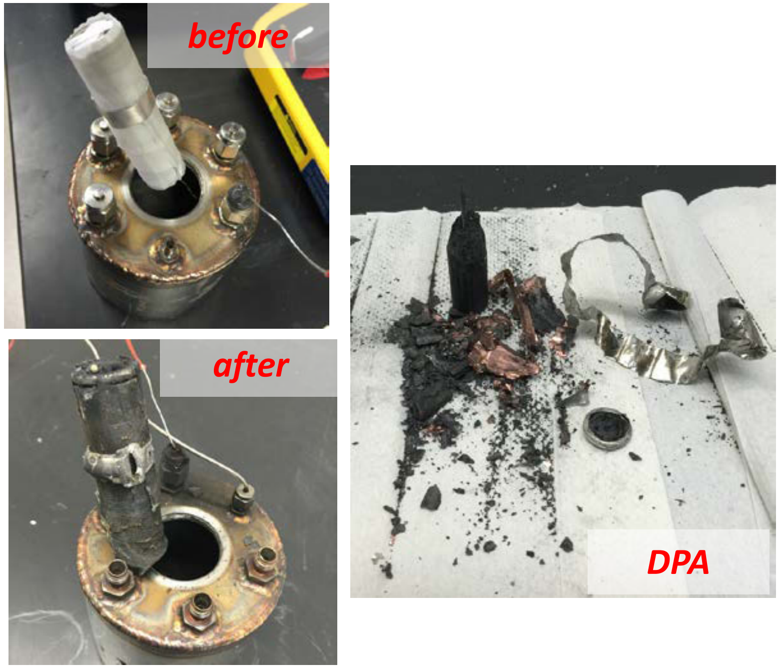
- NREL EDM – Fluent API

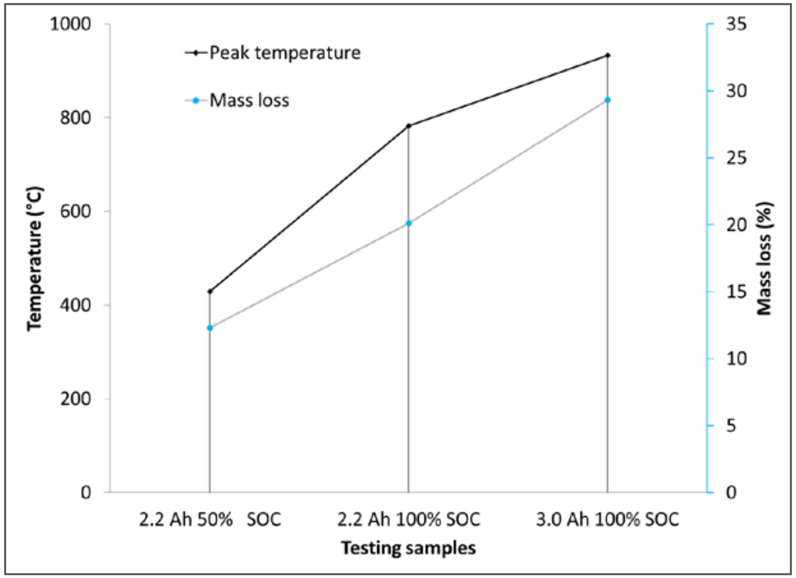
CDM

- SPPC CDM-electrothermal model in ANSYS® Fluent® MSMD-module

ARC Testing of NMC 18650 Cells

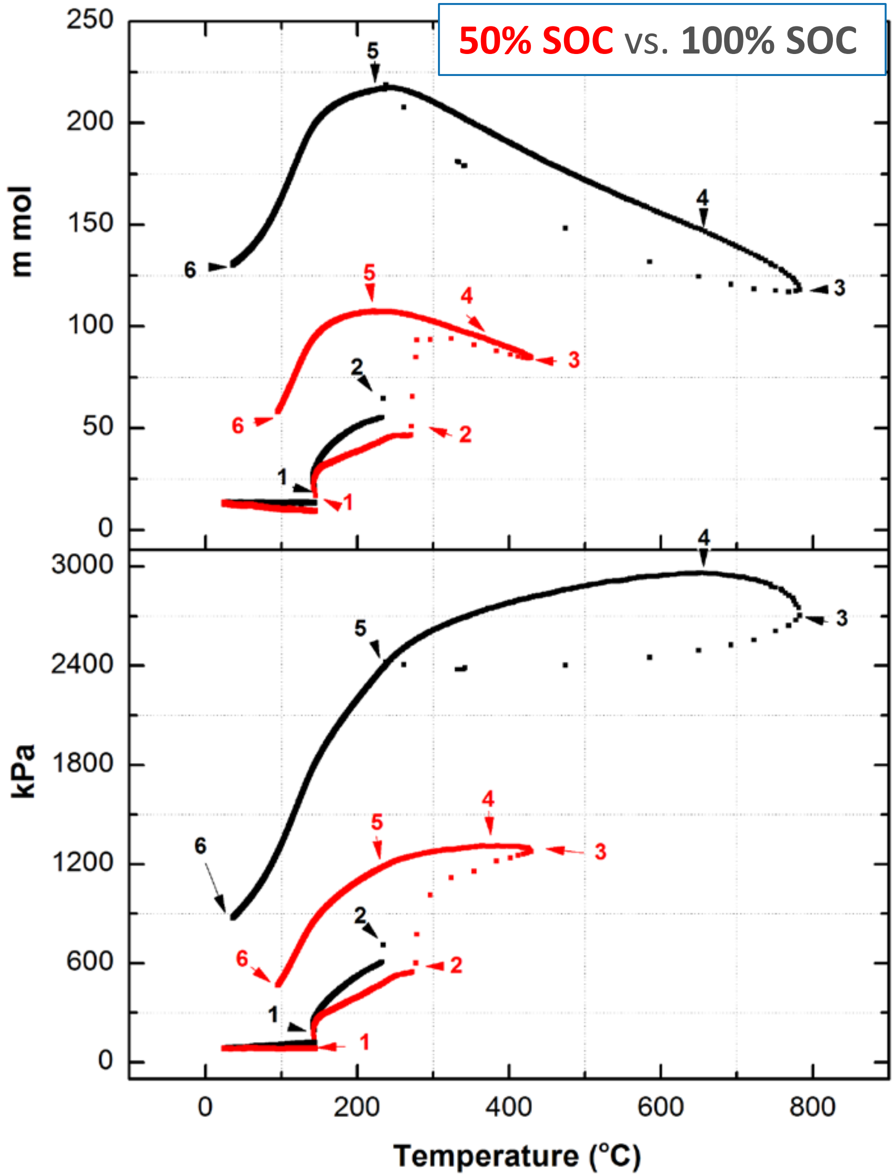






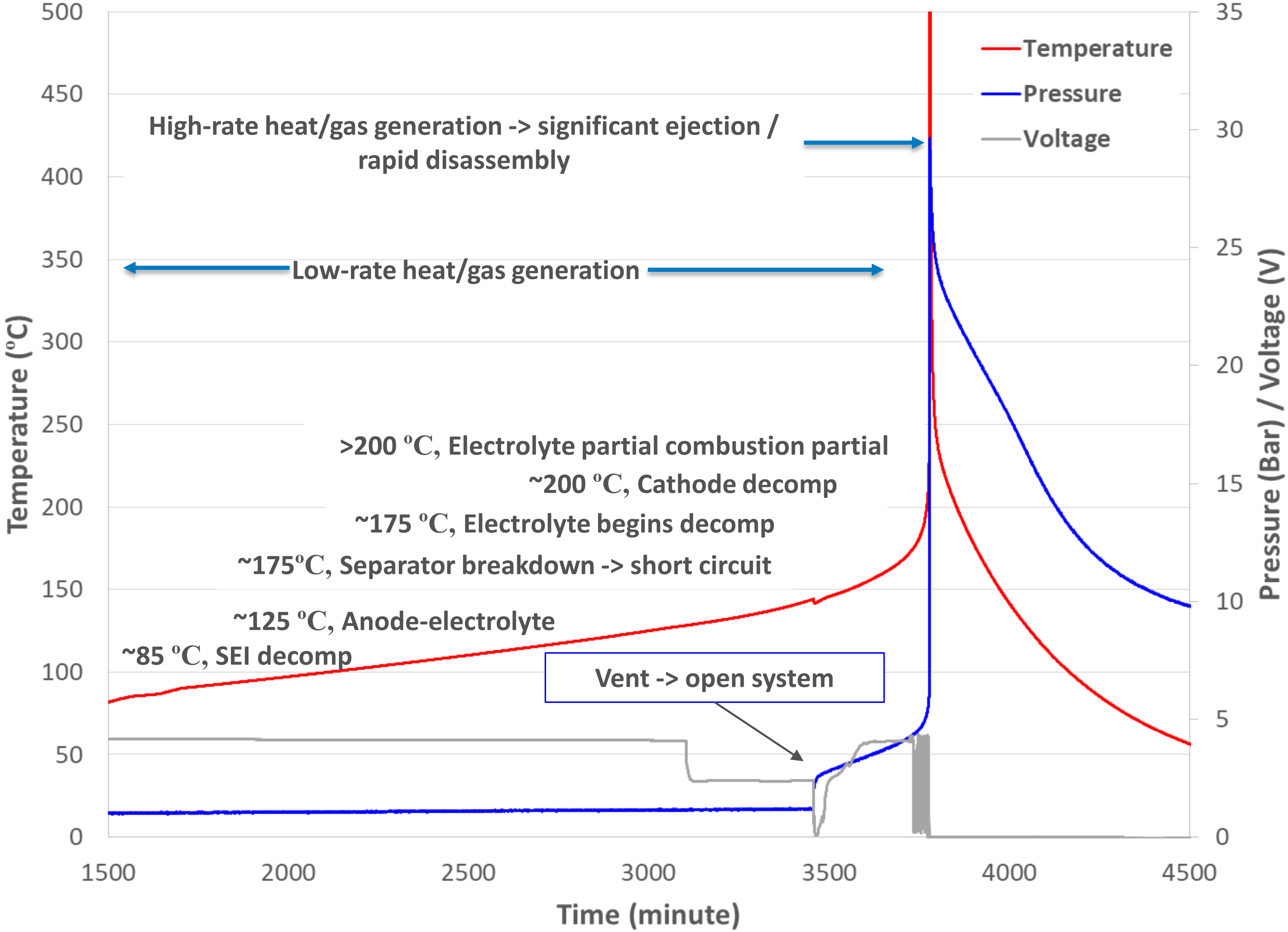
- Mass loss affected by cell SOC and volumetric energy density
  - Might associated with peak temperatures
- Ejecta includes gases, solids and fluids. DPA reveals substantial melting of aluminum current collector, ejected out of the can.

Gas Generation Analysis



- Chronological order
  - Vent opened (1) → Rapid TR (2) → Max temperature (3) → Max pressure (4) → Max amount of gas (5) → end (6)
- Measured pressure and temperature, calculated amount of gas generated
  - Assumed ideal gas behavior
  - Might not apply between 2 and 3 during very dynamic pressure change)
- Temperature measured on cell skin might not represent the real gas
- Gas generation continued after peak temperature
- High pressure hot gas condensed into liquid (5 →6).

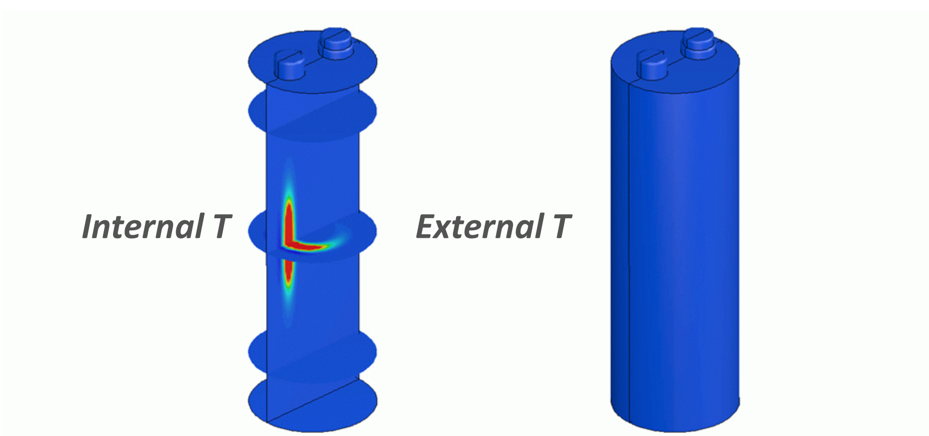
Reactions and Events during ARC Testing



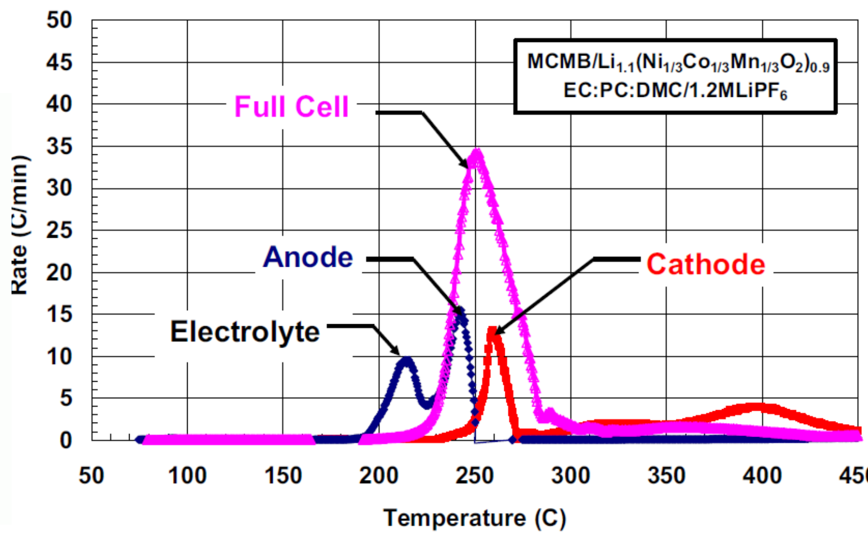
ARC Tests vs ISC Conditions

- ARC testing of cell components not providing all insights on full cell behaviors
- Battery responses to ARC testing and ISC conditions are different
  - **ARC testing**: cell-wide uniform response. Vent triggered by some solvent vaporization and SEI decomposition
  - **ISC**: local failure, gas generated by local electrolyte vaporization and decomposition reactions.

From components to full cells,
Superposition principle may not work



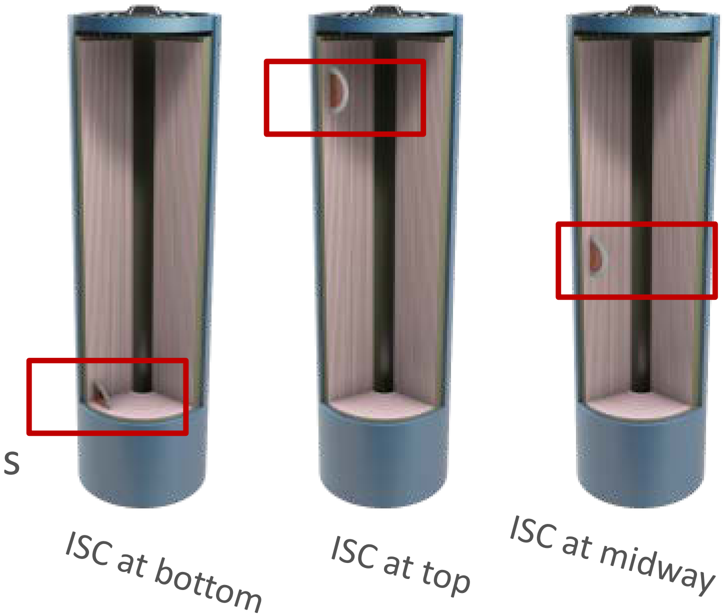
Local defects -> ISC -> local hot spot -> gas generation

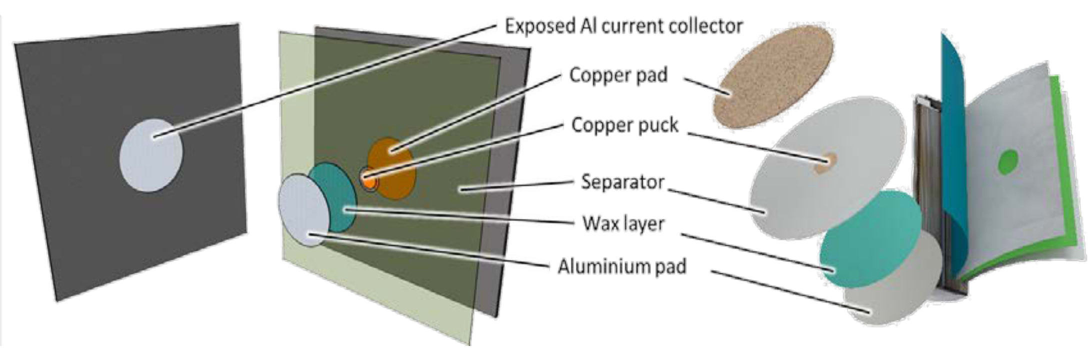


E.Peter Roth, SNL ECS Transactions 11(19)2008

Identifying Worst-Case Failure Scenarios

- Investigated by NASA JSC, NREL and UCL
- Vary the location of the internal short circuiting (ISC) device to identify worst-case failure scenarios
  - likely to cause side-wall ruptures
  - likely to cause vent clogging and bursting
- 18650 cells were manufactured with the ISC device placed at 3 different longitudinal locations at 2 different radial depths





Internal short circuiting device

Bursting and breach at top

Modeling Thermal Stress and Bursting Pressure

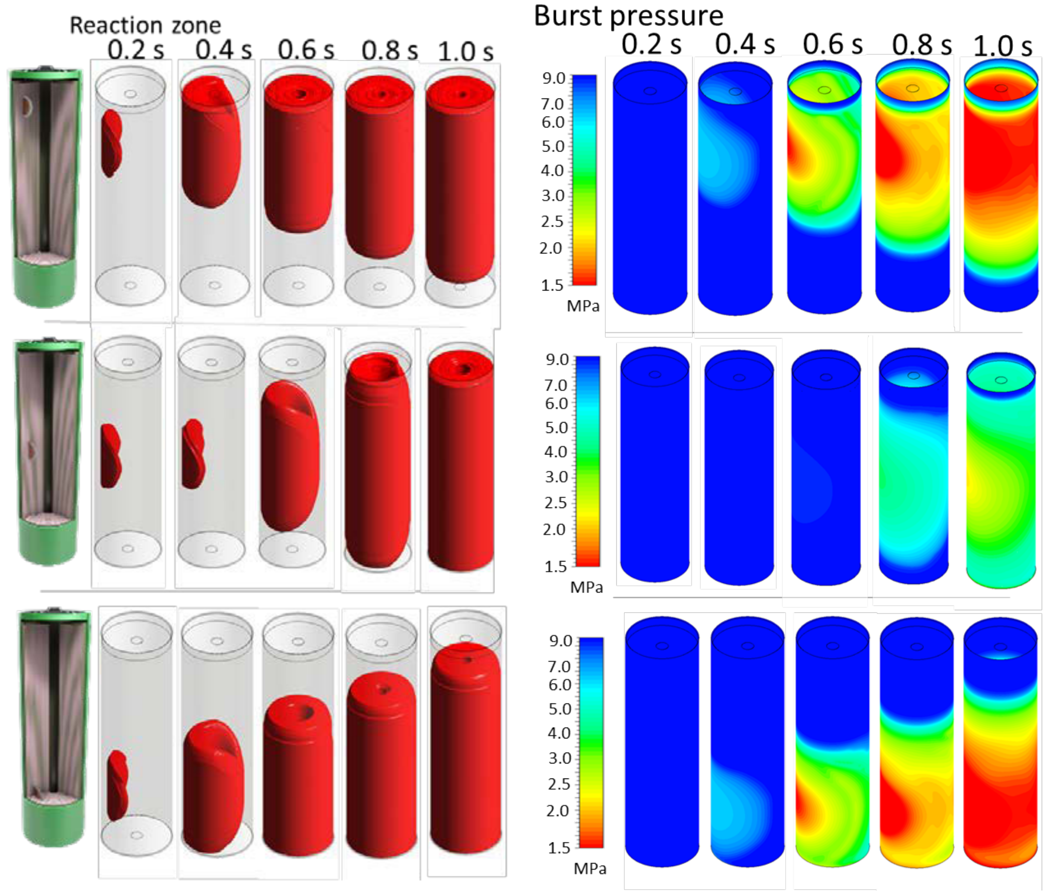
Journal of Power Sources 417 (2019) 29–41

Modelling and experiments to identify high-risk failure scenarios for testing the safety of lithium-ion cells

Donal P. Finegan[a,*], John Darst[b], William Walker[b], Qibo Li[a], Chuanbo Yang[a], Rhodri Jervis[c], Thomas M.M. Heenan[c], Jennifer Hack[c], James C. Thomas[b], Alexander Rack[d], Dan J.L. Brett[c], Paul R. Shearing[c], Matt Keyser[a], Eric Darcy[b]

Reaction kinetics -> Can temperature -> Burst pressure

- Bust pressures can reach < 1.5 MPa for temperatures > 650 °C
- If a cell produces 6 L of gas, and is clogged, the internal pressure could reach 30 MPa
- Lower temperatures are reached for initiation at the middle. The highest risk scenarios for pressure-induced breaches are initiation of TR near end of the 18650 cell.



Based on temperature-dependent tensile strength properties for S350GD mild steel

Modeling External Hot Gas Flow

Step 1: Internal gas flow modeling

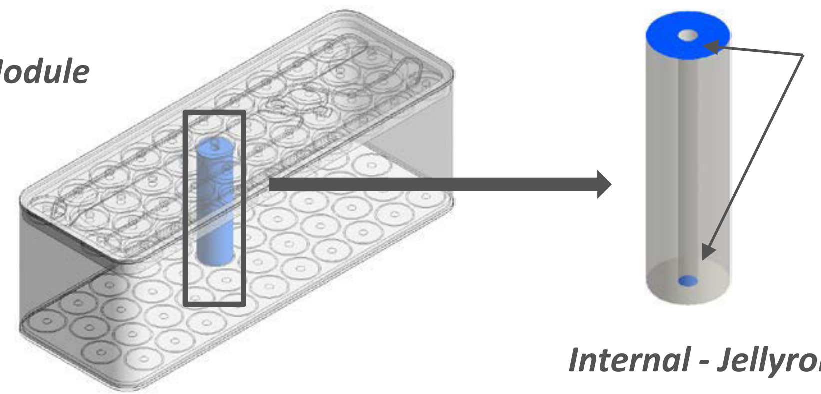
Single jellyroll (JR)
With fine mesh

→ Single jellyroll abuse simulation (i.e. internal short circuit)

→ Criteria allowing sequential modeling approach

↓

<u>Output</u>
Reaction conversion &
Heat generation rate



↓

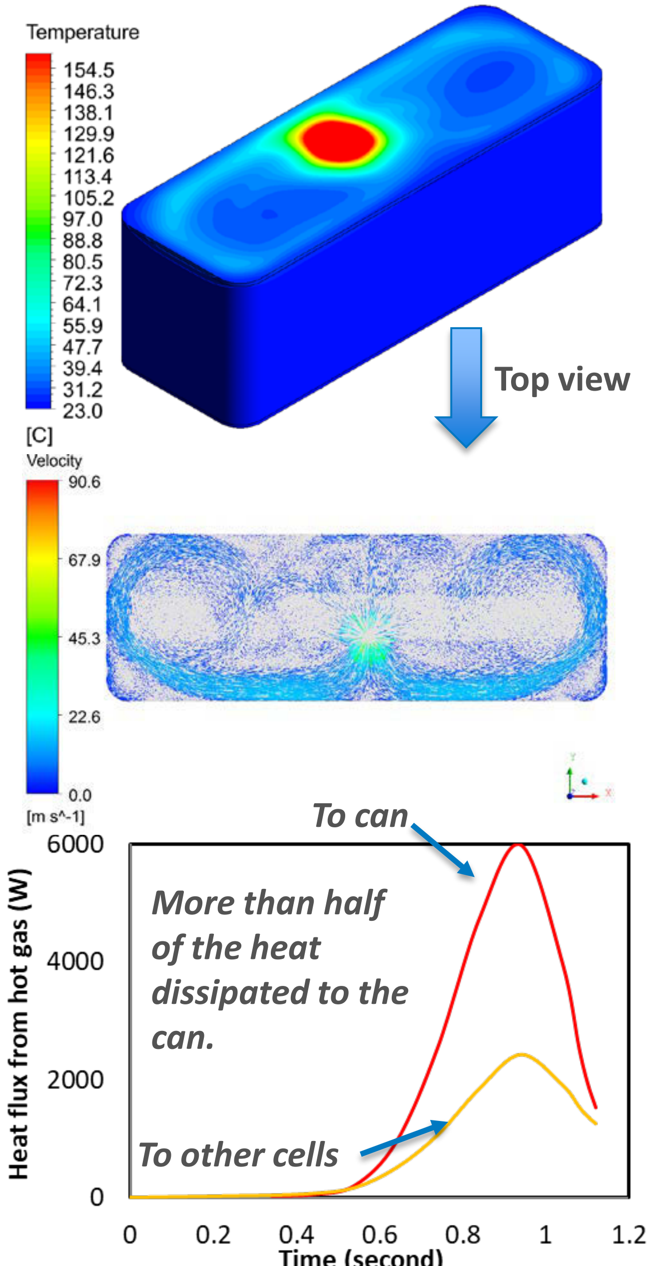
Gas generation rate
Heat generation rate

← Module-level venting simulation

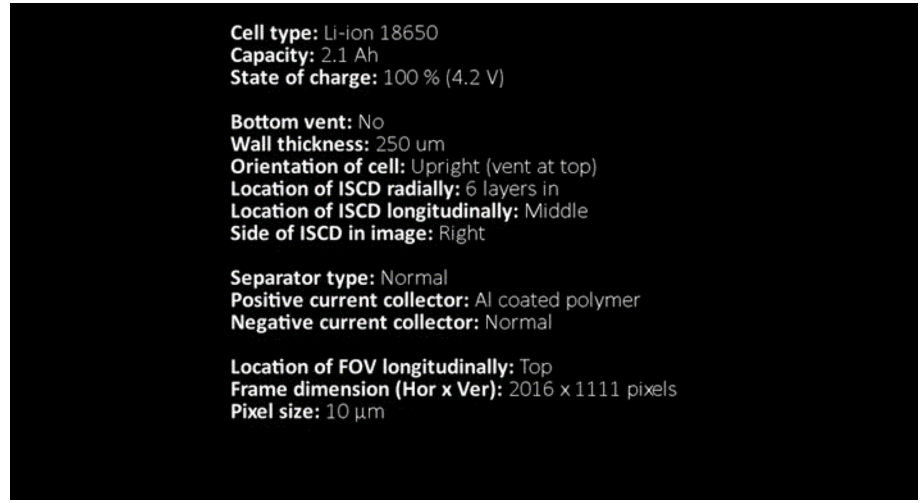
← <u>OUTPUT</u>
Temperature, pressure and velocity distribution during the abuse event

Step 2: External gas flow modeling

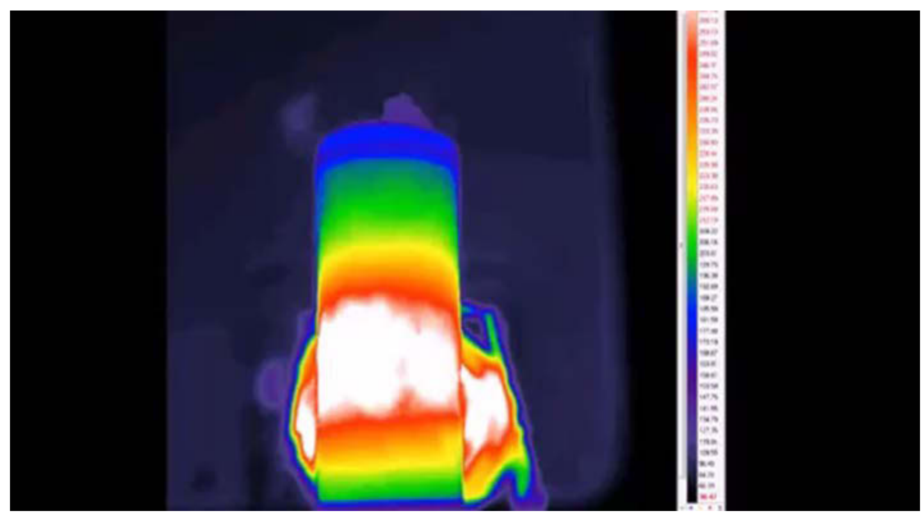
Mass and Heat Transfer in Ejection



Mass Ejection

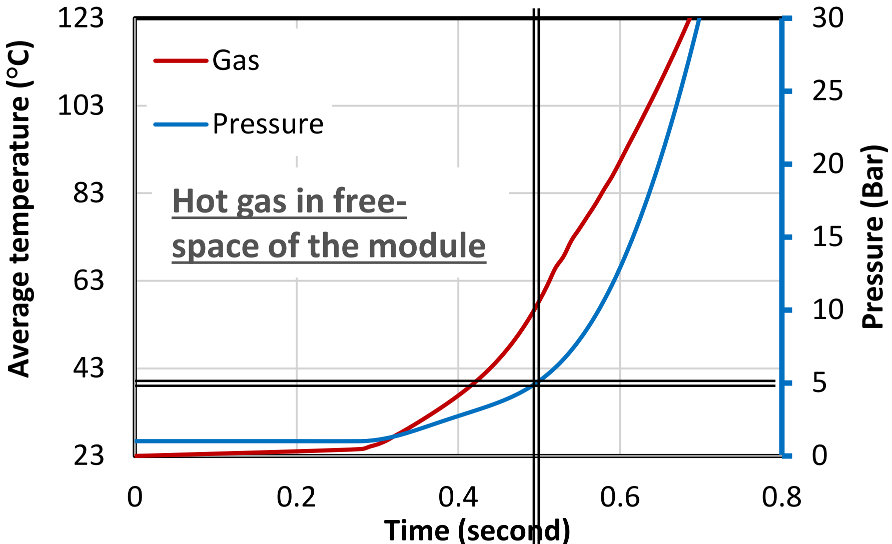


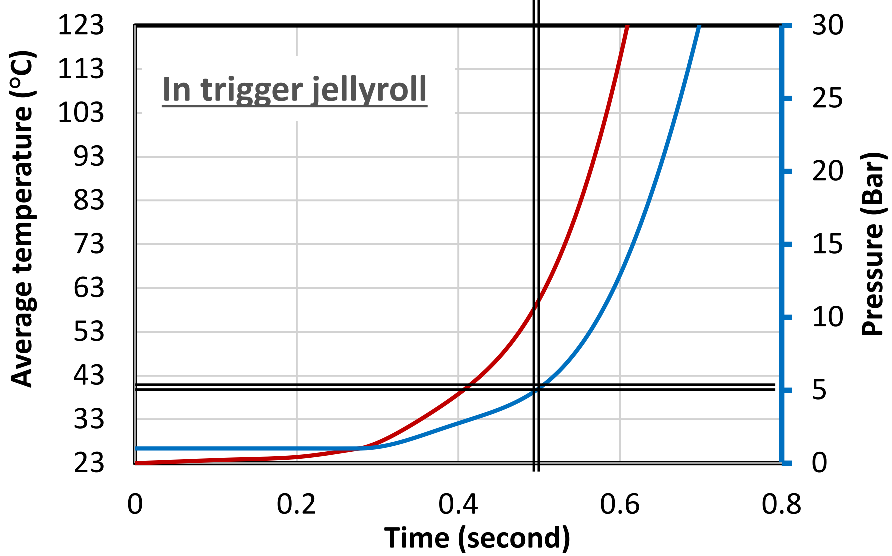
Heat Ejection



Video credits: NREL– Donal Finegan

Vent Pressure and Cell Conditions



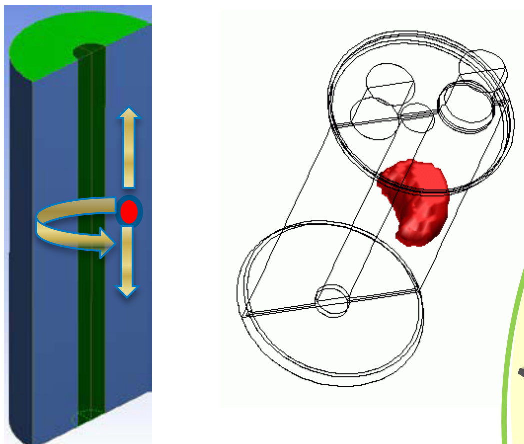


- Results correlate module safety vent design with single cell transient failure
- Left figures show a example to use modeling results for vent design
  - If the vent opens at 5 bar, temperatures of hot gas in the trigger cell and module free space are both 40 ºC respectively
  - Gas generated due to local thermal runaway within the ISC jellyroll can trigger the vent despite that average jellyroll temperature rises moderately.

Gas Kinetics in 18650 Cells (Ongoing)

ISC Modeling Study

- Multiphysics ISC modeling
- Understanding behaviors



- *Confirm Model Assumptions*
- *Provide Model Input*

Model Validation

Experiment Design

ISC Experimental Study

Cell type: Li-ion 18650
Capacity: 3.4 Ah
State of Charge: 100 % (4.2 V)
Bottom vent: Yes
Wall thickness: 220 µm
Orientation of cell: Positive end up
Location of ISCD radially: 6 winds in
Location of ISCD longitudinally: Middle
Side of ISCD in image: Right

Location of FOV longitudinally: Middle
Frame rate: 4869 Hz
Frame dimension (Hor x Ver): 1616 x 616 pixels
Pixel size: 10 µm

- *Identify Critical Parameters*
- *Provide Complete Data Set for Non-Measurable Quantities*

High speed x-ray video credits:
NREL– Donal Finegan

Summary

- An integrated safety modeling approach established under CAEBAT project
- The safety model can be used as a predictive tool for battery pack safety engineering
  - Its functionality was demonstrated with thermal runaway mitigation tests
- For high energy cells, mass and heat transfer through ejection becomes significant. Gas kinetics model is being incorporated in the integrated approach to address these behaviors
  - A sequential approach is suggested for module-level simulation
- Combined techniques including multi-physics modeling, calorimetry, ISC devices, high-speed X-ray imaging and thermal imaging enhance understanding of battery safety behaviors.

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