Thermal Abuse Modeling of Li-Ion Cells and Propagation in Modules

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Outline

Methodology for Understanding Impacts of Battery Design Parameters on Thermal Runaway in Lithium-Ion Cells/Modules

- Background
- Objectives
- Simulating Internal Short in a Cell
  - Parametric runs
  - Results
- Propagation in a Module
- Summary

Background

- Last year, in LLIBTA-3, we introduced our approach for modeling Li-ion thermal abuse[1]
  - Chemical reactions at elevated temperatures
    - SEI decomposition
    - Negative-solvent reaction
    - Positive-solvent reaction
    - Electrolyte decomposition

    } Used literature information for graphite–cobalt oxide chemistry
  - Captured real 3-D geometries and boundary conditions
  - Performed oven heat test simulations
  - Simulated localized heating – cell internal short
  - Cell-to-cell propagation in a module
    - Balance between discrete heat sources and thermal network
    - Heat transfer through radiation, conduction, and convection

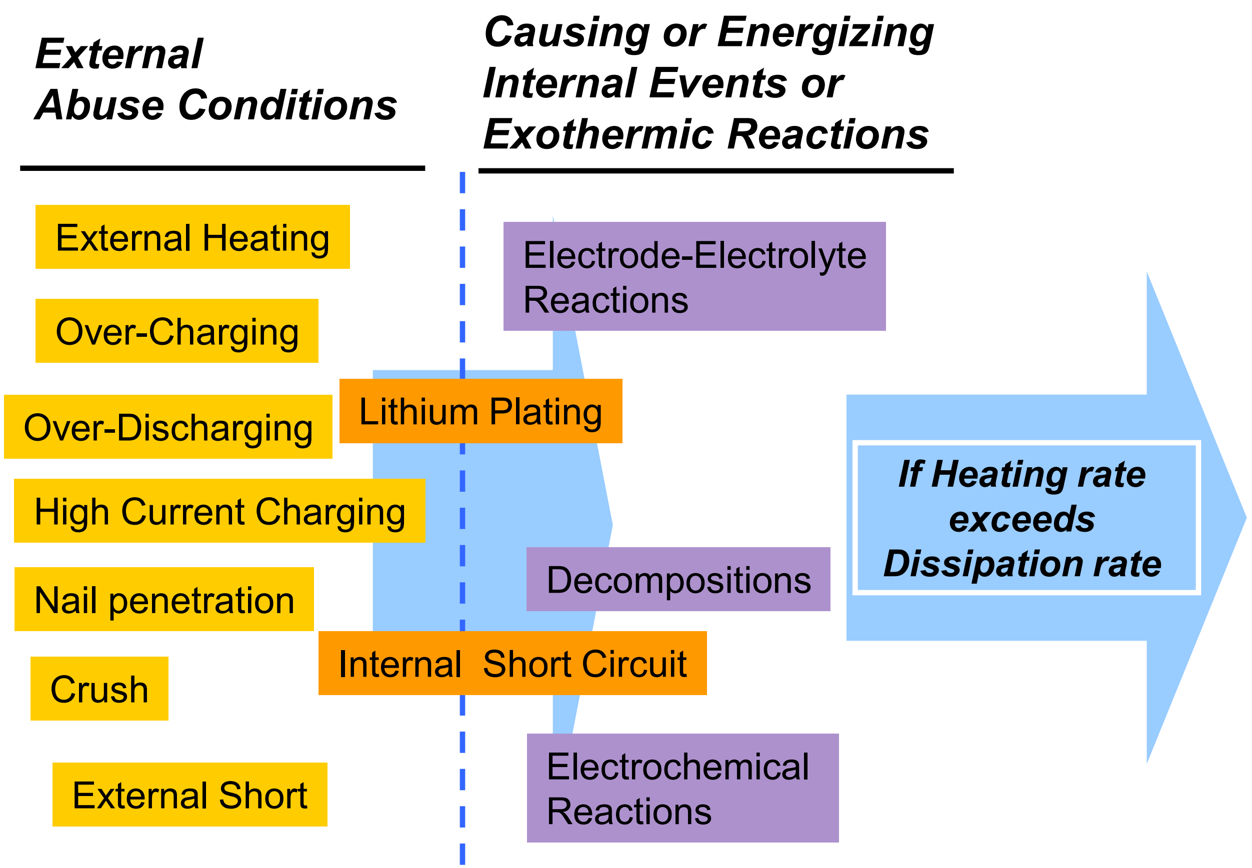
[1] G.-H. Kim, A. Pesaran "Analysis of Heat Dissipation in Li-ion Cells & Modules for Modeling of Thermal Runaway," 3rd Large Lithium Ion Battery Technology and Application, May 2007, Long Beach, CA

Thermal Runaway - Background

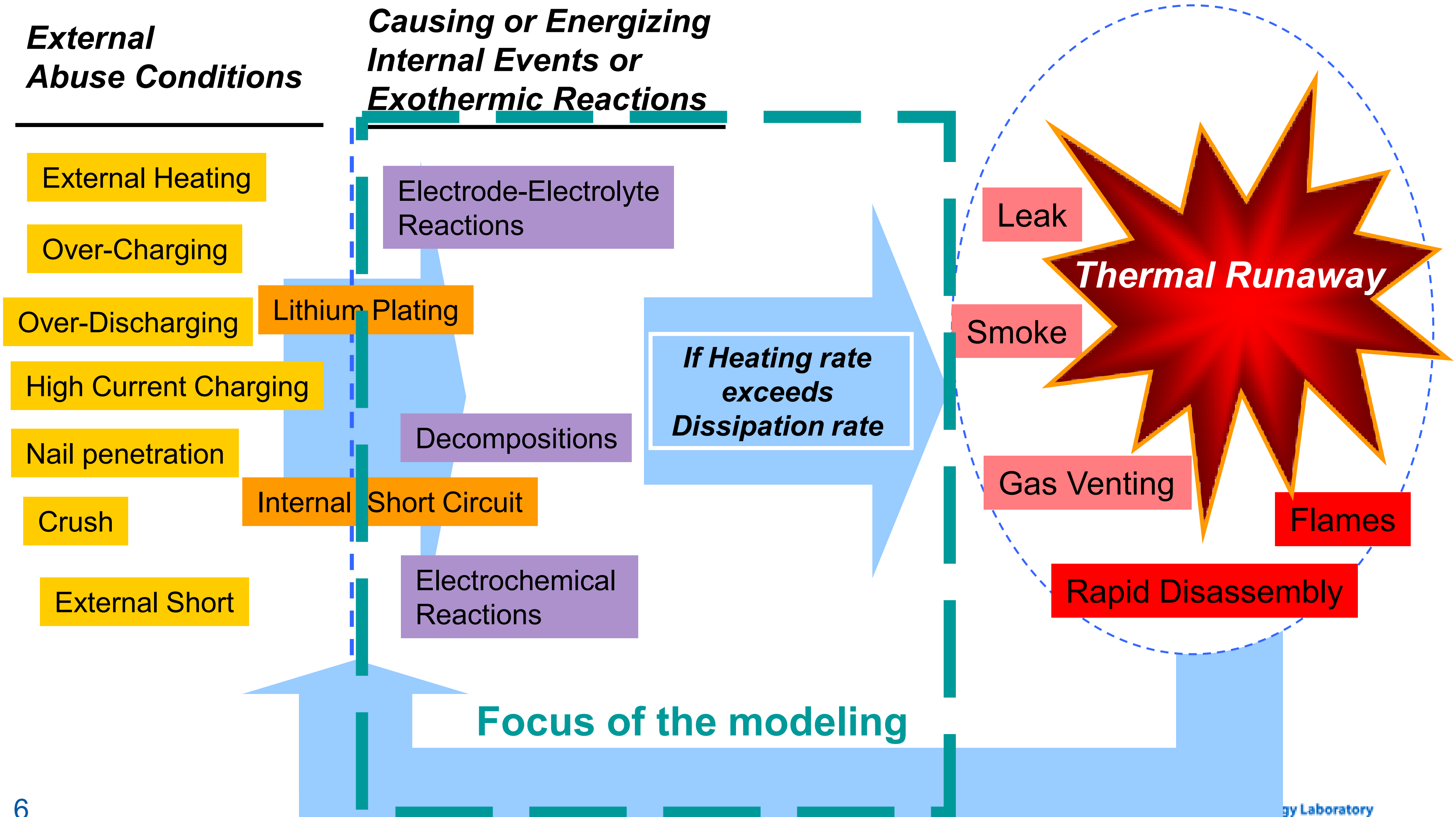
External Abuse Conditions

- External Heating
- Over-Charging
- Over-Discharging
- High Current Charging
- Nail penetration
- Crush
- External Short

Thermal Runaway - Background



Thermal Runaway - Background



Background - Approach

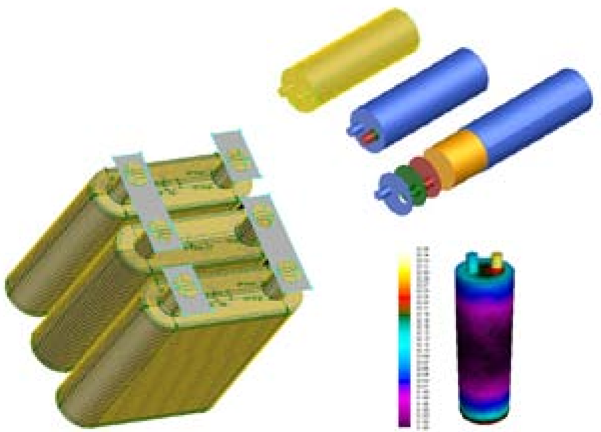
- Formulated *Exothermic Reactions* at elevated temperatures

> *Reproduce thermal abuse modeling of Li-ion cells provided by Hatchard et al. (J. Electrochem. Soc. 148, 2001);*
> *Bob Spotnitz provided insight for reaction formulation*

→ Component reactions were fitted to Arrhenius type reactions.
→ Kinetic parameters were determined from ARC/DSC literature data.

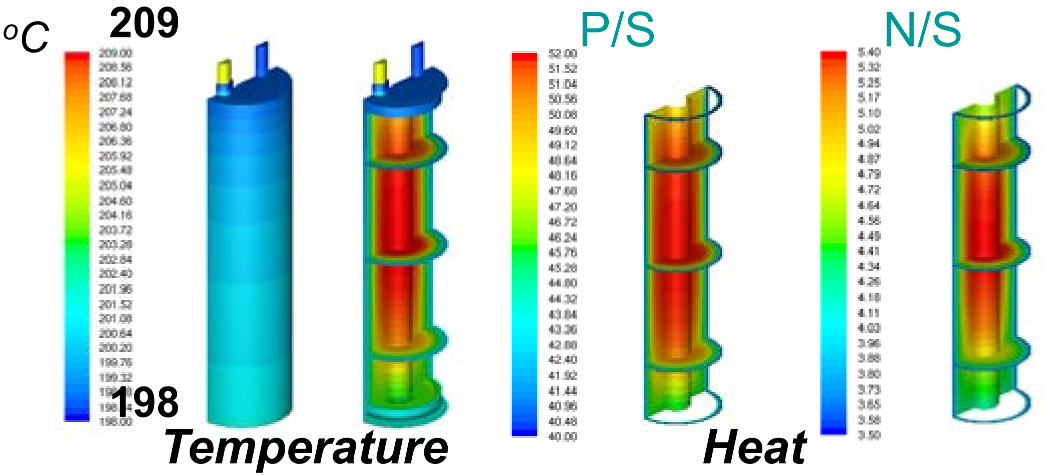
- Extended to *multi-dimensional models* capturing *actual thermal paths* and geometries of cells and modules.

→ A commercial finite-volume method (FVM) solver, FLUENT, was used.



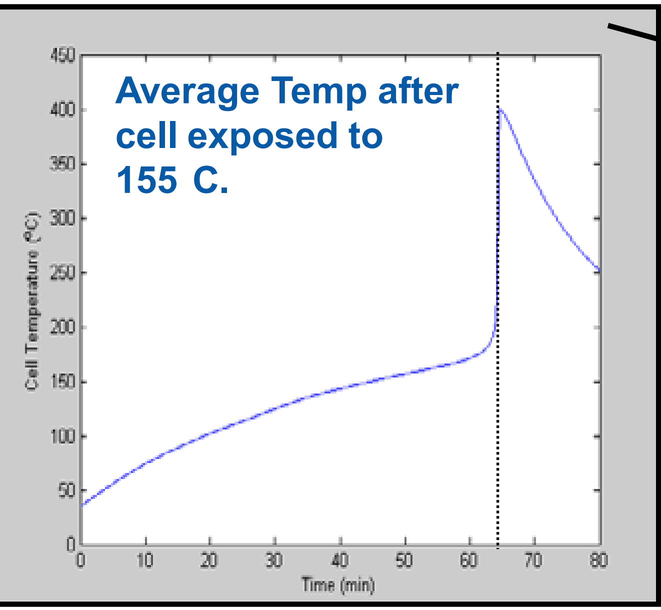
Background- 3D Oven Heat Test

Small Cell (D18H65)* *D18H65: Diameter of 18 mm, Height of 65 mm

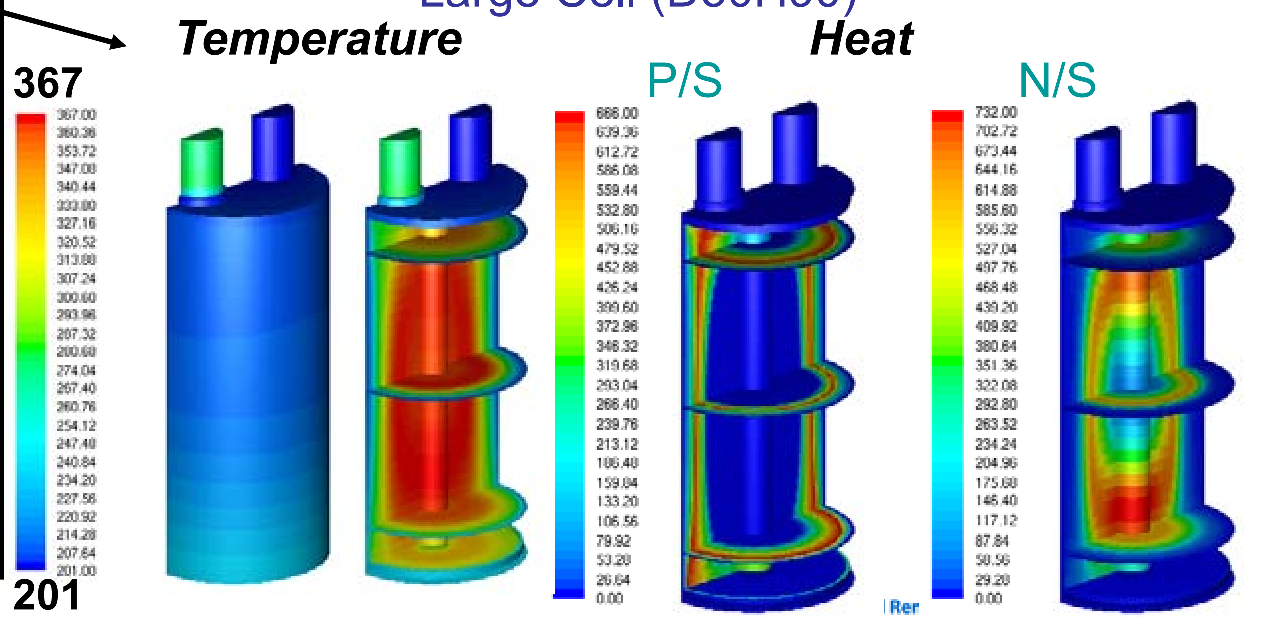


Although oven test is not a highly multidimensional phenomenon, it still demonstrates noticeable spatial distribution, especially in large cells.

P/S: positive/cathode-solvent
N/S: negative/anode-solvent



Large Cell (D50H90)



Objectives of this Study

Continue to explore thermal abuse behaviors of Li-ion cells and modules that are affected by local conditions of heat and materials

- Use the 3D Li-ion battery thermal abuse "reaction" model developed for cells to explore the impact of the location of internal short, its heating rate, and thermal properties of the cell.
- Continue to understand the mechanisms and interactions between heat transfer and chemical reactions during thermal runaway for Li-ion cells and modules.
- Explore the use of the developed methodology to support the design of abuse-tolerant Li-ion battery systems.

Cell Level Thermal Runaway Analysis

- **Internal Short Simulation**
  - ✓ Impact of short location in a cell
  - ✓ Impact of thermal property of cell materials
  - ✓ Impact of heating rate at short event

Model Description

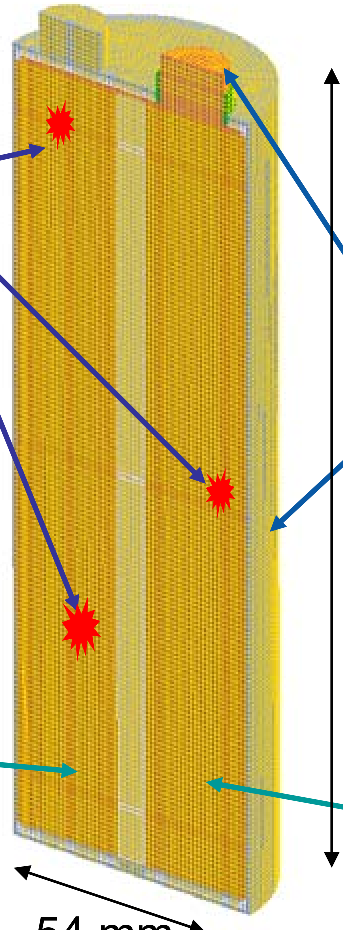
½ Model with Symmetry Plane

Hot-Spot

- Localized energy is released in a short period of time in a very small volume of the core.
  - Initially we assumed 5% of stored electric energy released
- Simulation of details of initial process of short is challenging, but we are trying to predict what happens after short happens.

Heat Sources

- Exothermic reaction heat
- No resistive/Joules heating



- MESH
  - ✓ Computational grid: 200K
  - ✓ Grid size: ~1 mm by 1 mm by 1 mm
  - ✓ Max: 2.01 mm^3 ; min: 0.31 mm^3

Thermal Boundary Conditions

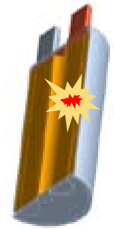
- Natural/forced convection
- Gray-body radiation

Core Material

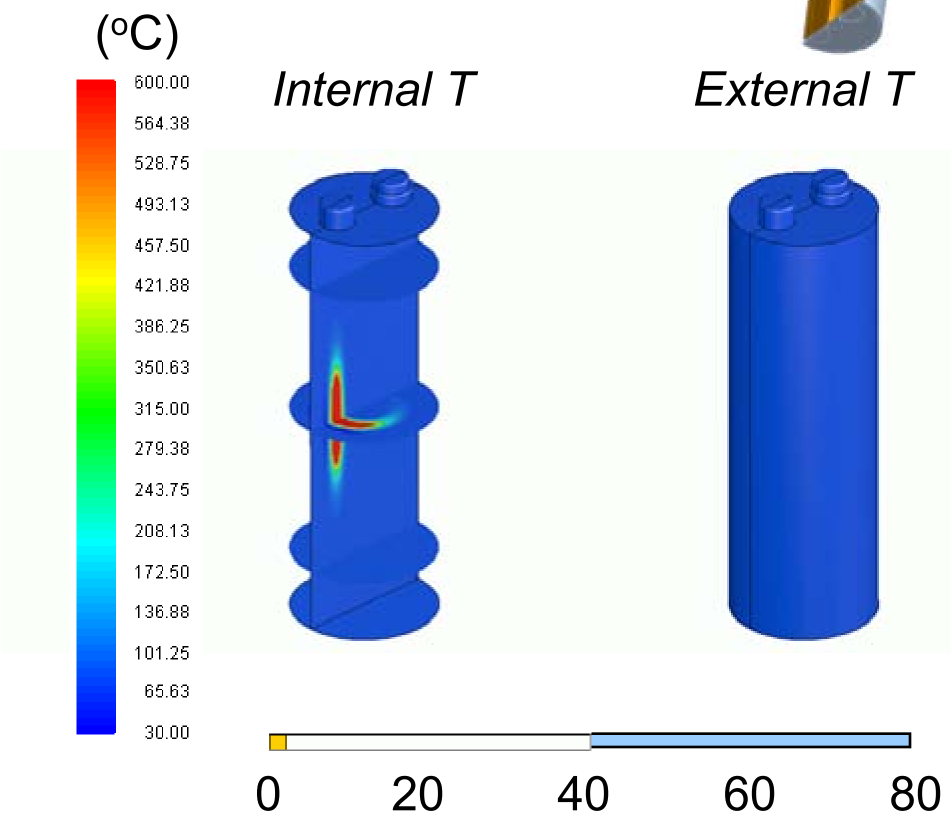
- Cylindrically orthotropic properties

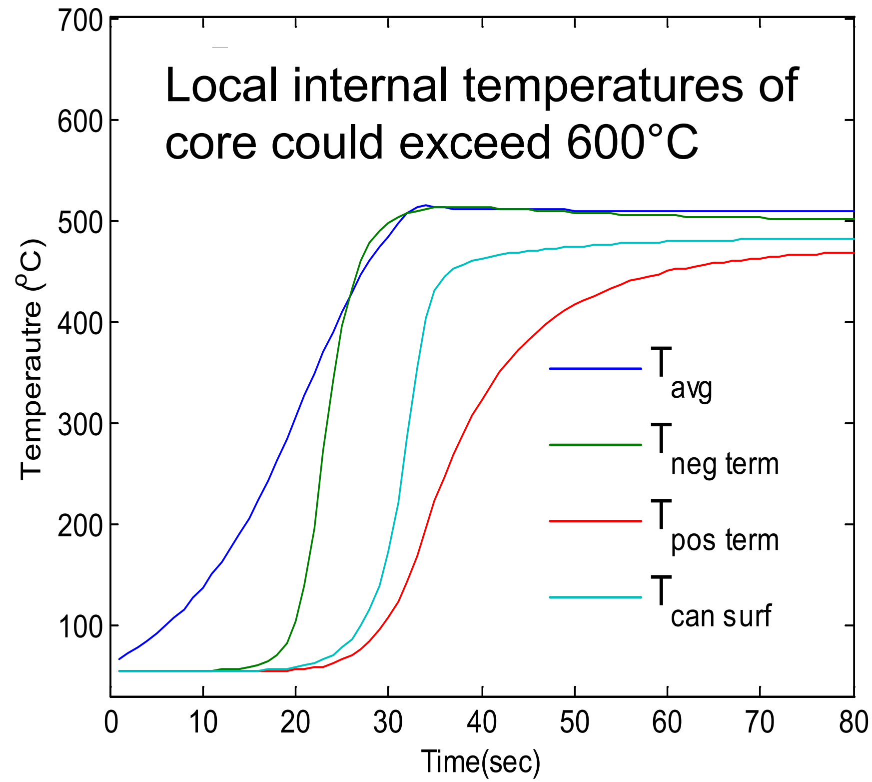
Temperature Evolution after a Short

Short in the middle of cell



5% of stored electric energy released in a short time at a small portion of active volume.





Delay between measuring external temperature and internal event, external sensing may be too late.

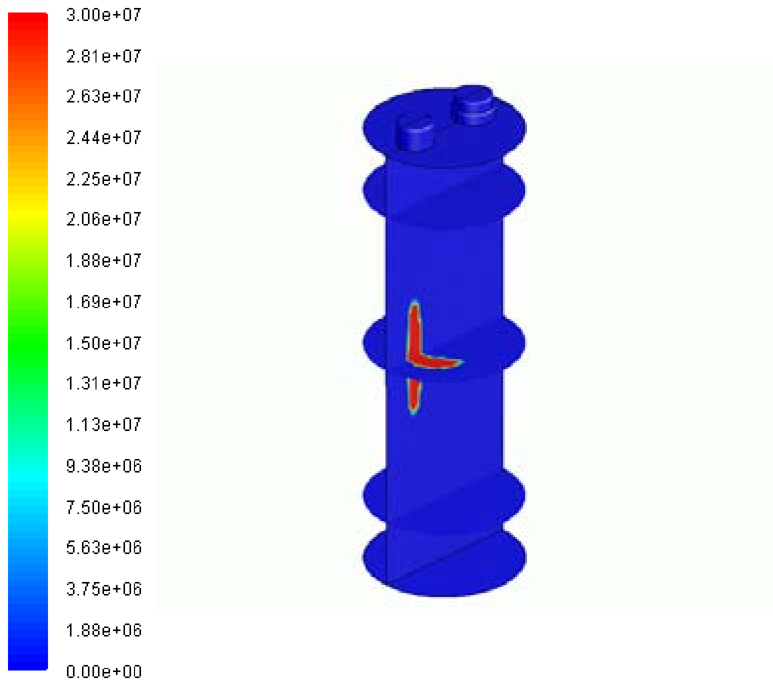
Volumetric Heat Generation after a Short

(Total and due to various reactions, showing how reactions propagate)

5% of stored electric energy released in a short time at a small portion of active volume.

(W/m^3)

Total heat



SEI decomposition

Positive/electrolyte

Negative/electrolyte

0 20 40 60 80 (sec)

Impact of the Location of the Short

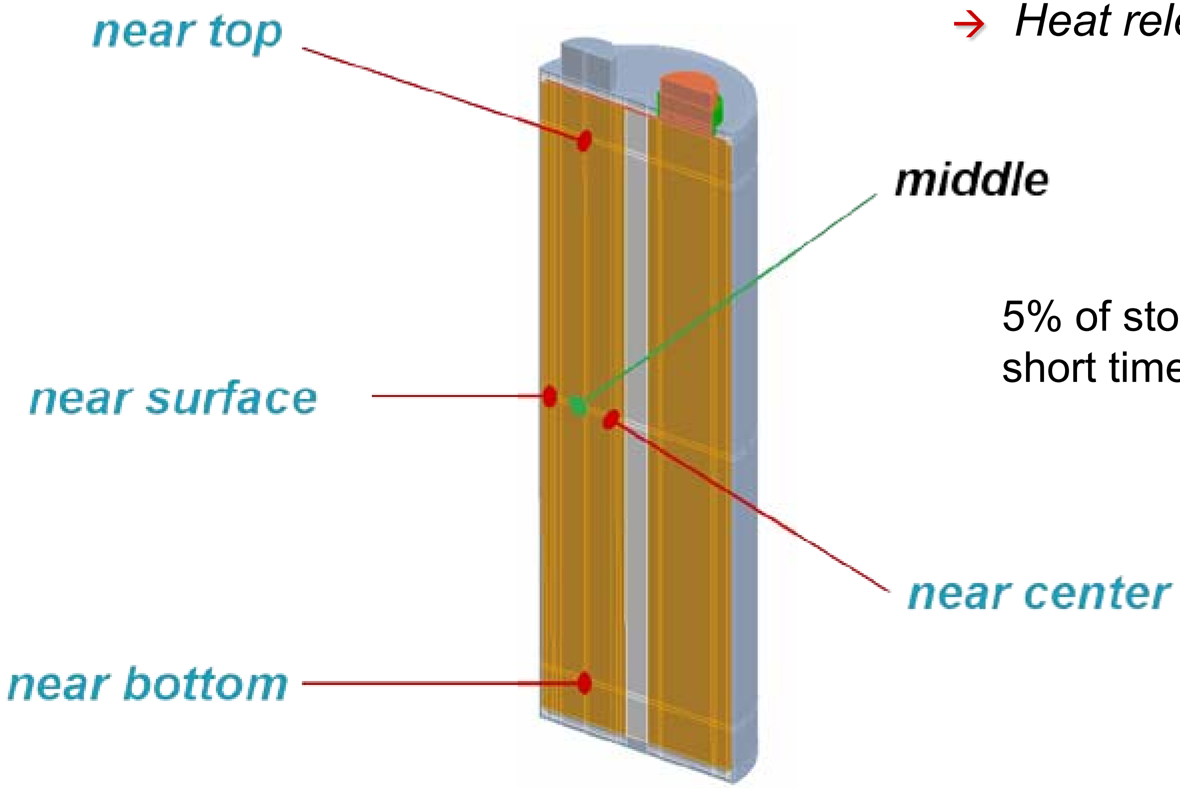
Layered structure of electrodes

→ *Preferred directions of reaction propagation*

Initial location of short and thermal paths and material distributions

→ *Propagation pattern*

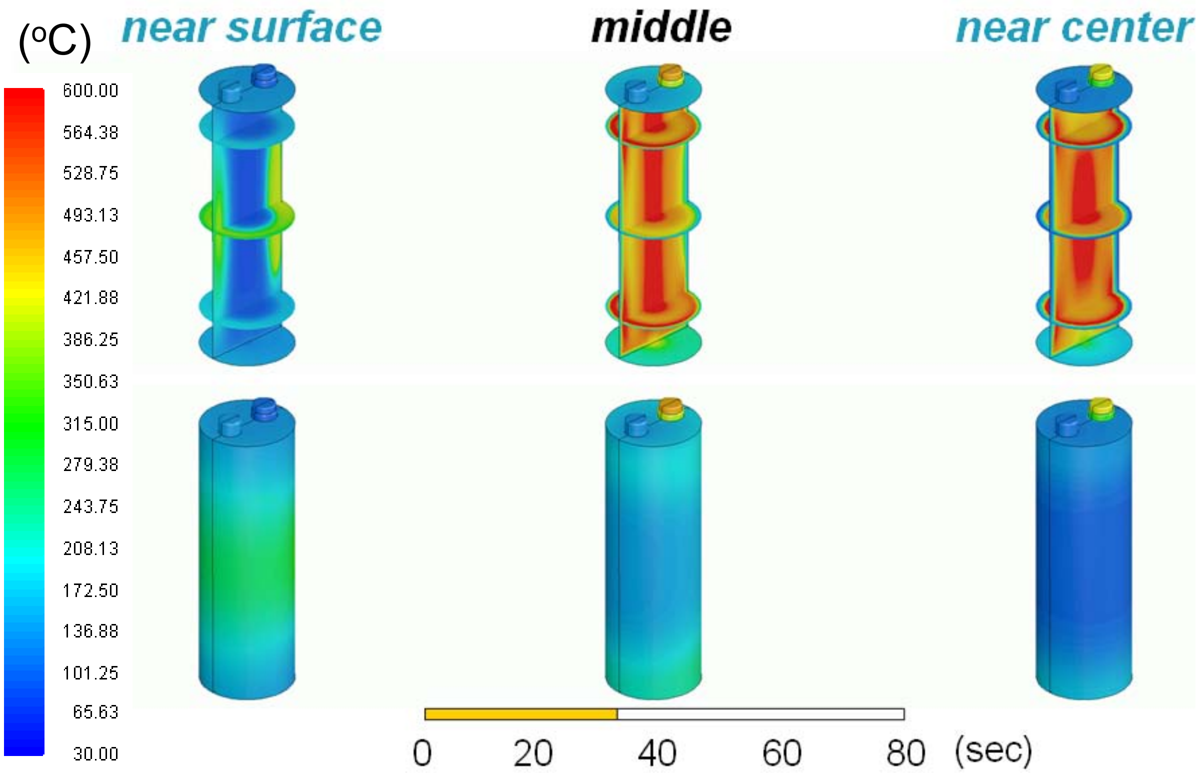
→ *Heat release duration*



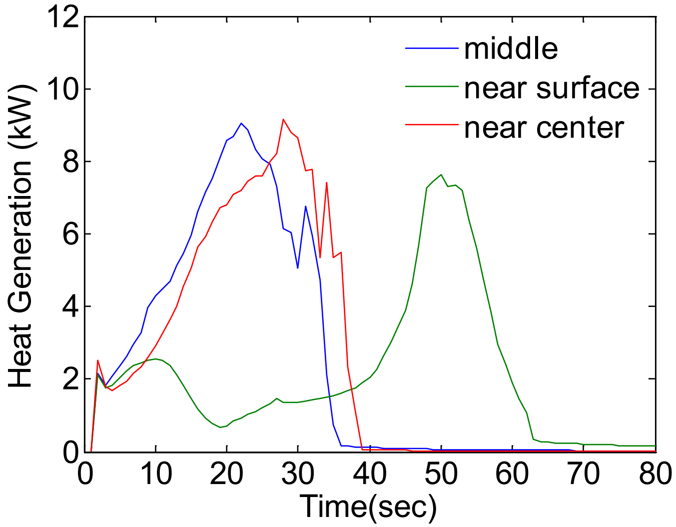
5% of stored electric energy released in a short time at a grid point.

Short Near Exterior Surface vs. Short Near Center of Cell

Heat dissipation is dependent on the location of heat release and thermal paths.



Snapshots of temperature distribution at interior (top) and surface (bottom) 38 seconds after short

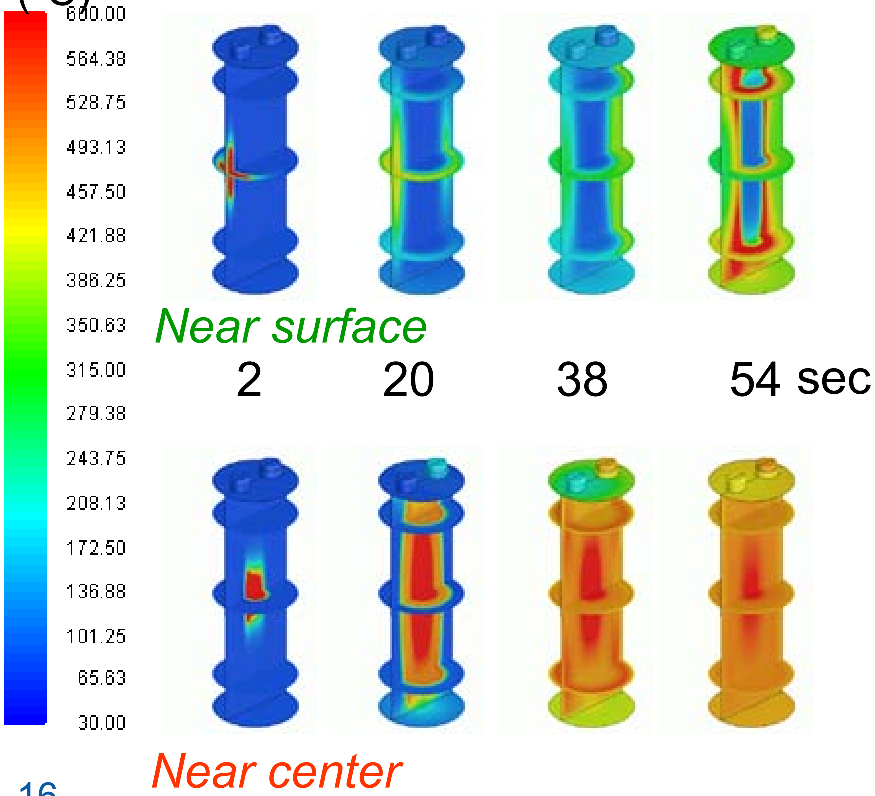


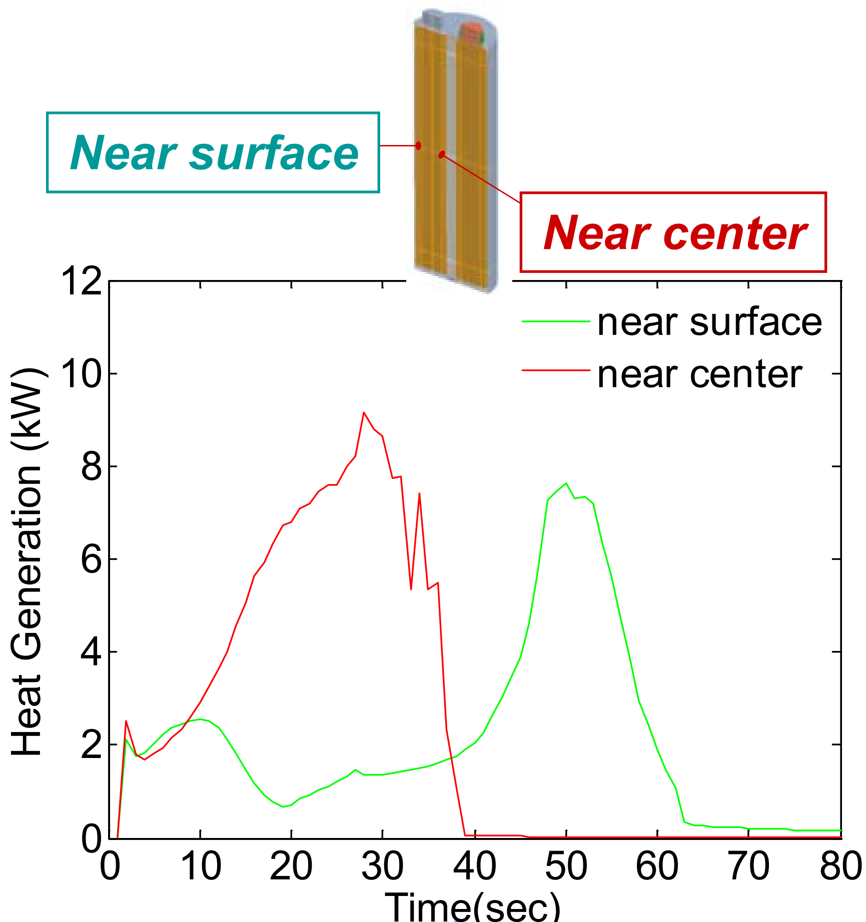
Total heat released (area under each curve) is about the same for three cases.

Short Near Surface vs. Near Center

- *Location of short has impact on how heat flows and abuse reactions propagate (e.g., delay in abuse reaction heat release for near-surface case).*

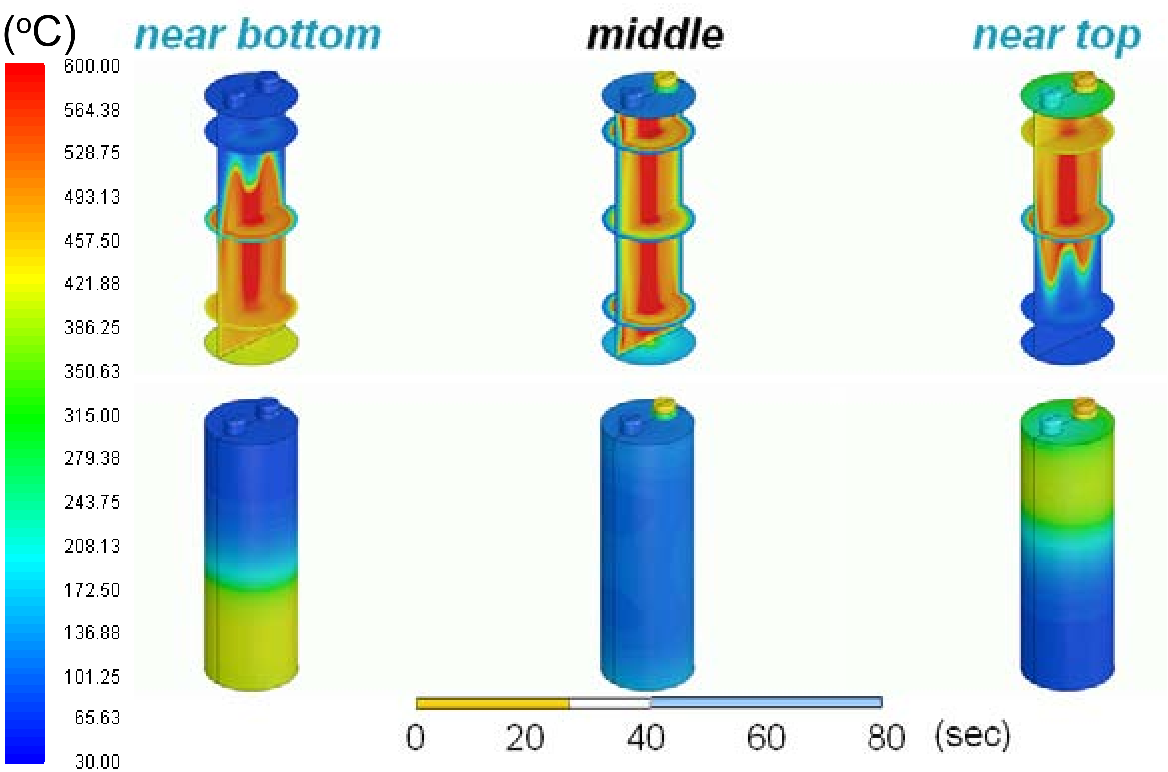
Temperatures (°C)



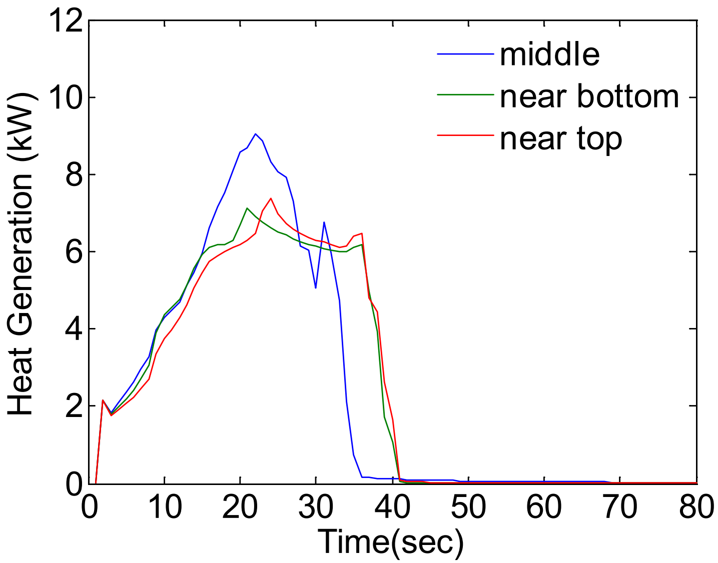


Short Near Bottom of Cell vs. Short Near Top of Cell

Heat dissipation is dependent on the location of heat release and thermal paths.



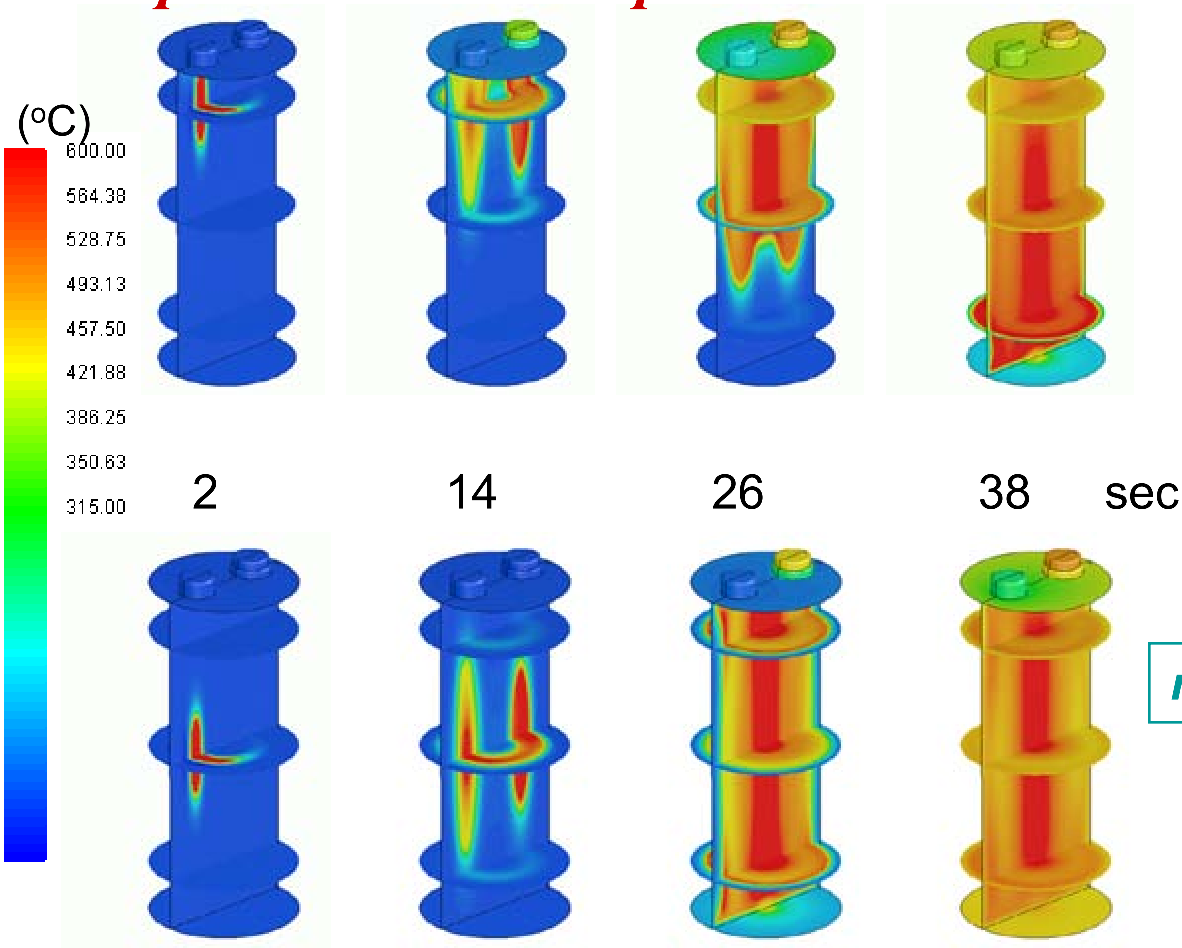
Snapshots of temperature distribution at interior (top) and surface (bottom) 25 seconds after short



Total heat released (area under each curve) is about the same for three cases.

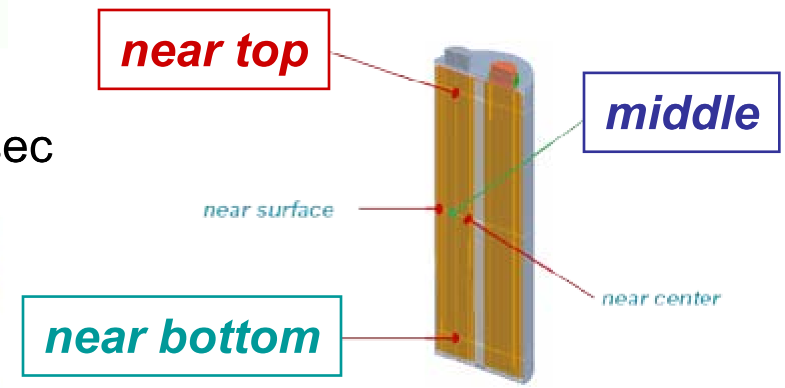
Short near top .vs. Short near bottom

Temperatures: near-top short



Temperatures: middle short

Heat dissipation is dependent on the location of heat release and thermal paths.



Impact of Thermal Properties

Heat Capacity

5% less ← C_p → 5% more

Thermal Conductivity

50% less ← k → 50% more

Electrode/current collector thicknesses and relative amount of component materials

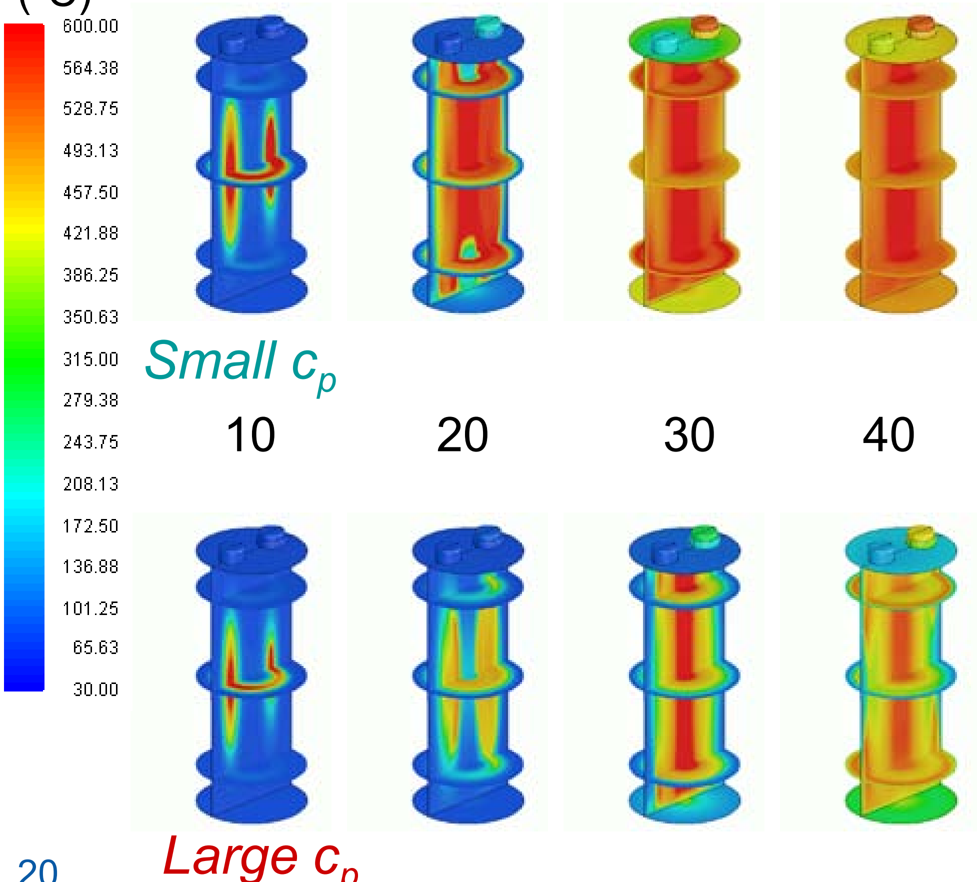
→ *Volumetric heat generation*

→ *Thermal properties of electrode sandwich*

Heat Capacity Impact on Cell Thermal Runaway

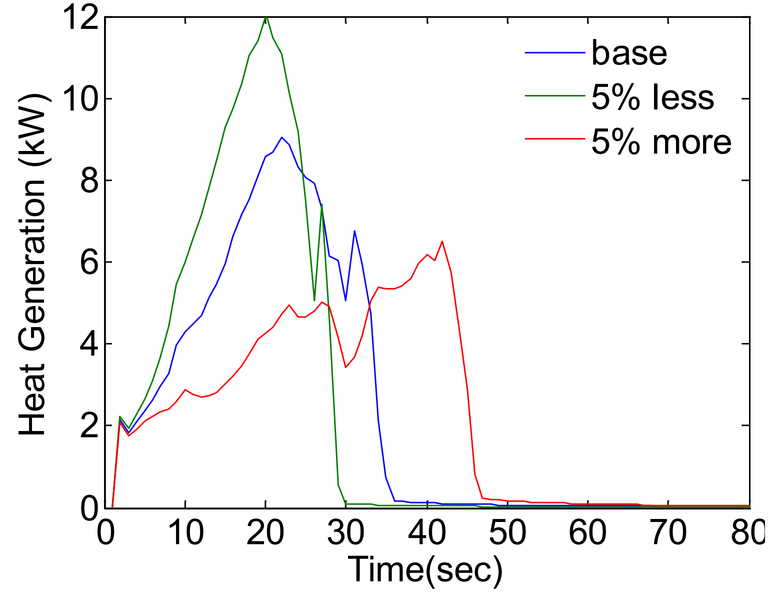
Reaction propagation is faster in a cell with smaller heat capacity.

Temperatures



Heat Capacity

5% less ← C_p → **5% more**

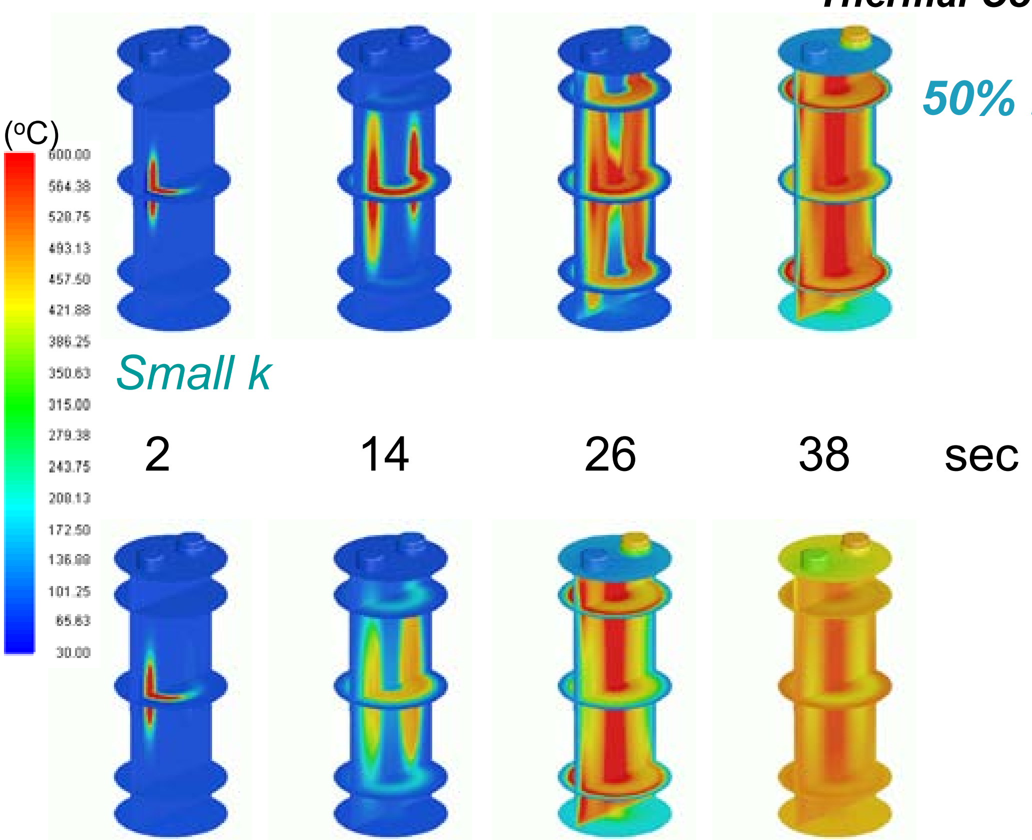


5% of stored electric energy released in a short time at a small portion of active volume.

Core Thermal Conductivity Impact on Cell Thermal Runaway

Reaction propagation is slower in a cell with smaller thermal conductivity

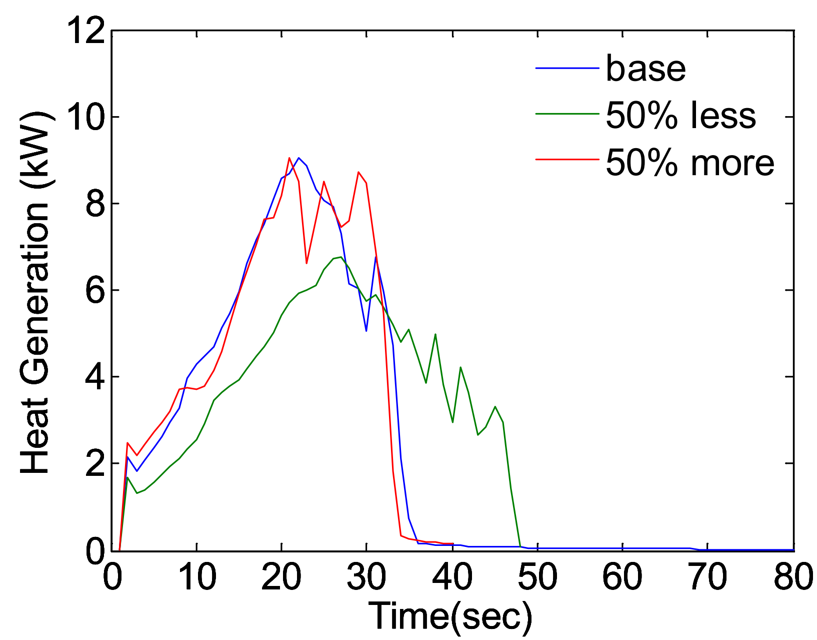
Temperatures



Large k

Thermal Conductivity

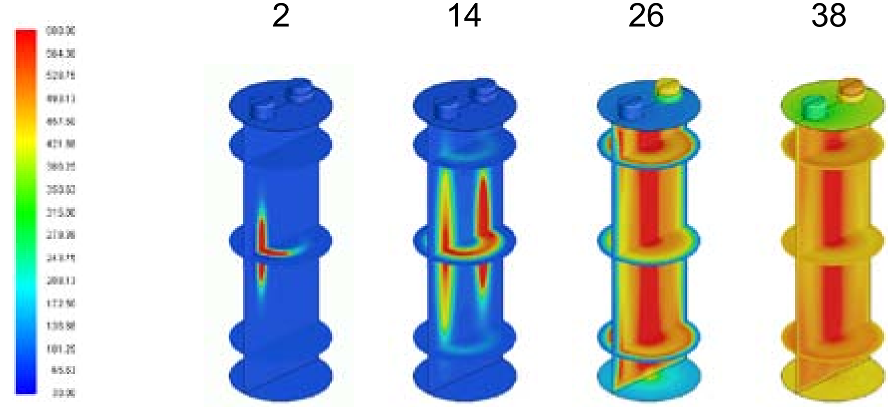
50% less ← *k* → **50% more**



Impact of Amount of Released Heat

Heat: % of cell energy release at a very small volume 1% ← 5%

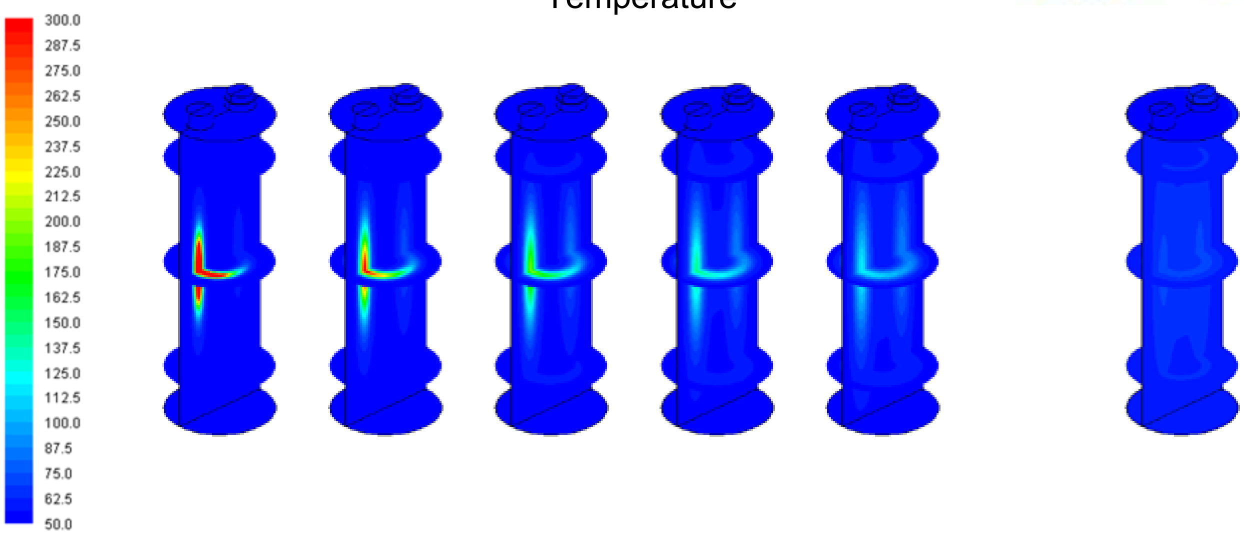
2 14 26 38



No thermal runaway with smaller heat release

Heat dissipates quickly without triggering thermal runaway.

(°C) Temperature



4 sec 8 sec 12 sec 16 sec 20 sec 60 sec

Pattern of initial heat release at short events need to be investigated.

We did an in-depth analysis.

Impact of Heating Rate in Short Events

Heat Release at a Short Event is affected by†

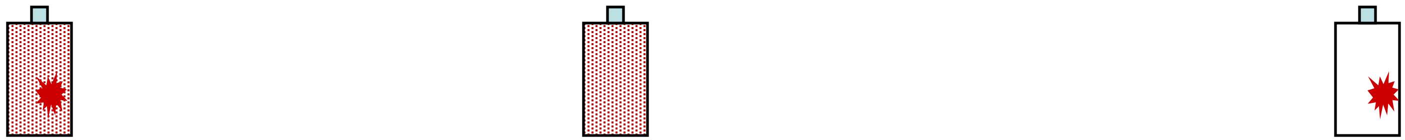
- Electrical Resistance of the Short
- Cell Power Rate (Power/Energy ratio)
- Cell Size (Capacity)

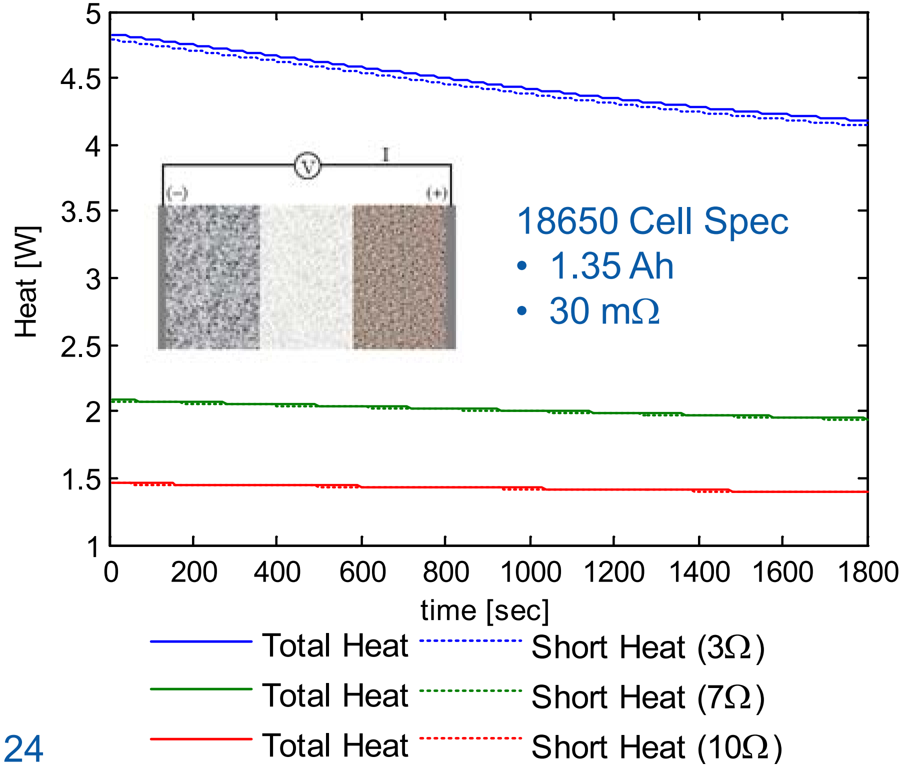
†This is based on our ongoing analysis and the details are beyond scope of this presentation. The next few slides look at a case with high-resistance short. Details of low-resistance case will be presented at other upcoming conferences.

Quantifying Heat Release at Short Event

Using Electrochemical Cell Model

Total Heat [W] **=** Volumetric Heat for Current Production + Heat Release at Short (***Short Heat***)





High-resistance Short Cases (3Ω, 7Ω, 10Ω) Observed from SNL Data

- Short current is determined by the short resistance rather than by the power rate or by the size of a cell.
- Relatively low c-rate for high resistance shorts
- Volumetric heat from current production is small
- Most released heat is local to the short site

Thermal Behavior of a Cell

at High-Resistance Short Events

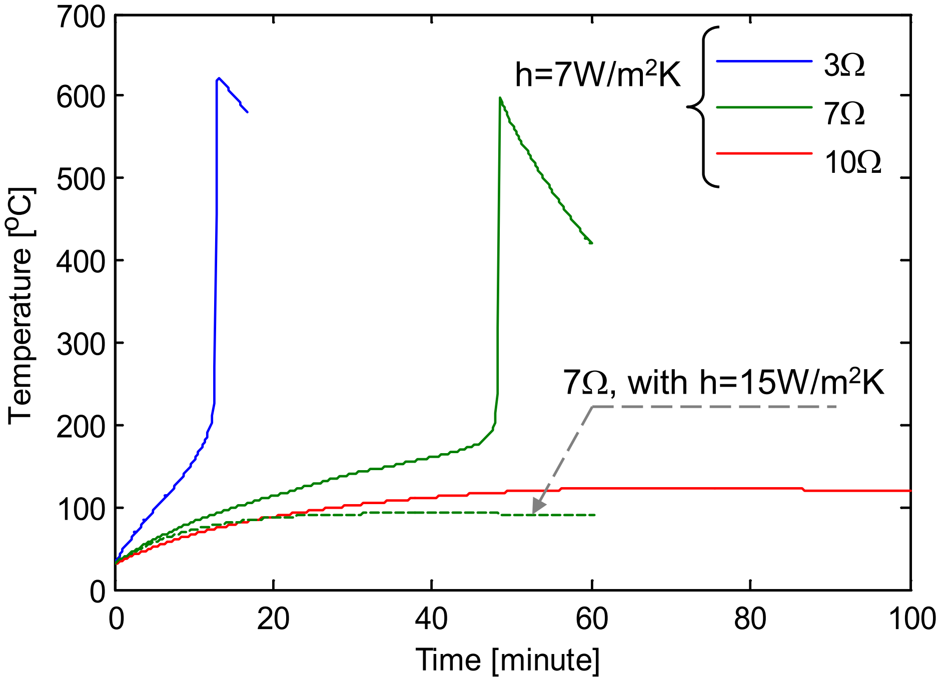
18650 CoO_2/graphite

30°C ambient, heat transfer coefficient on cell surface (h) = 7 W/m^2K

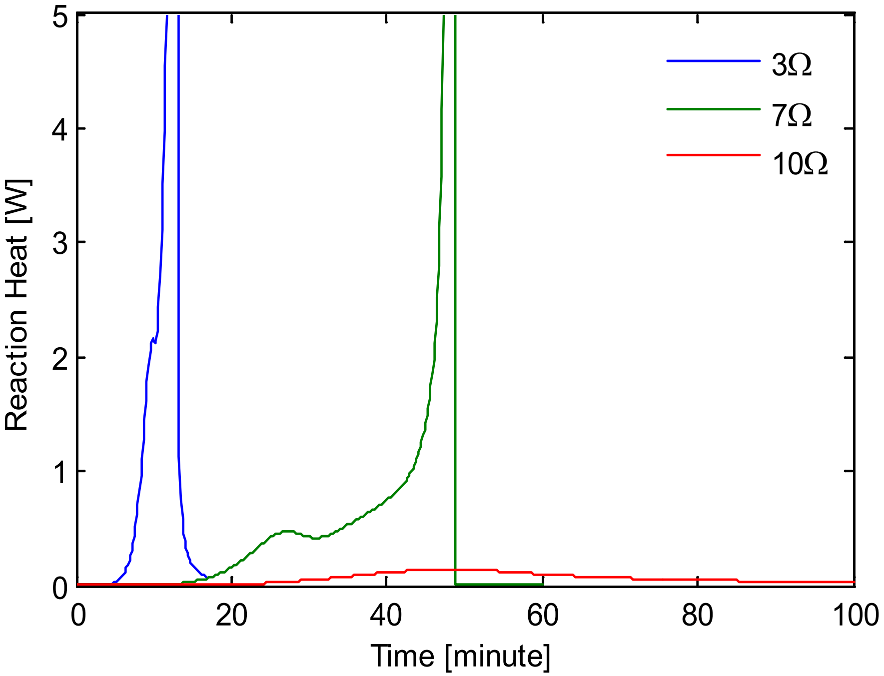
Strong natural convection in air

Heat Dissipation vs Heat Release

Temperature

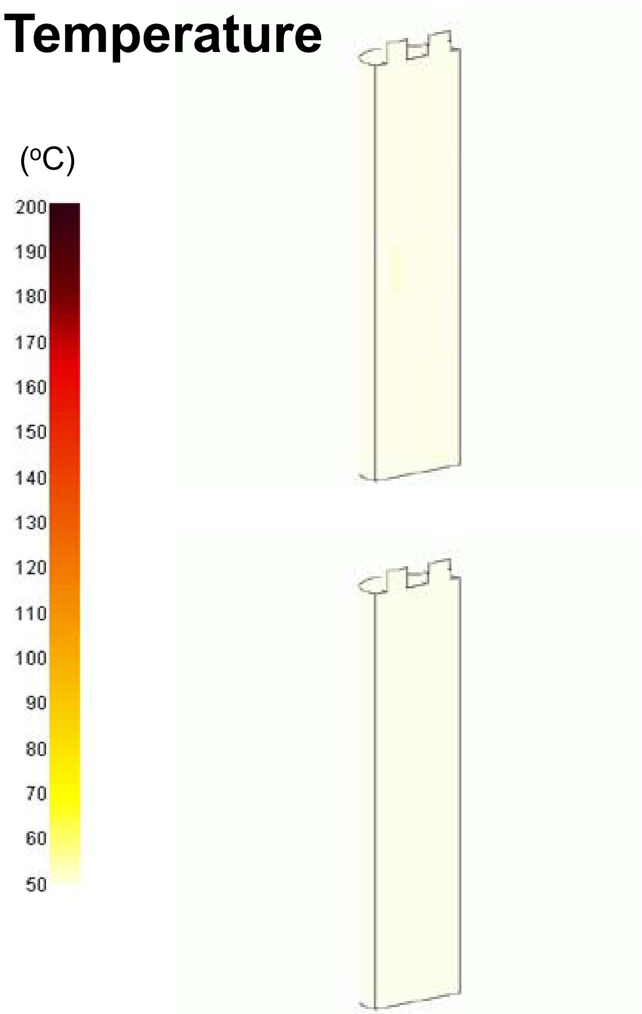


Reaction Heat



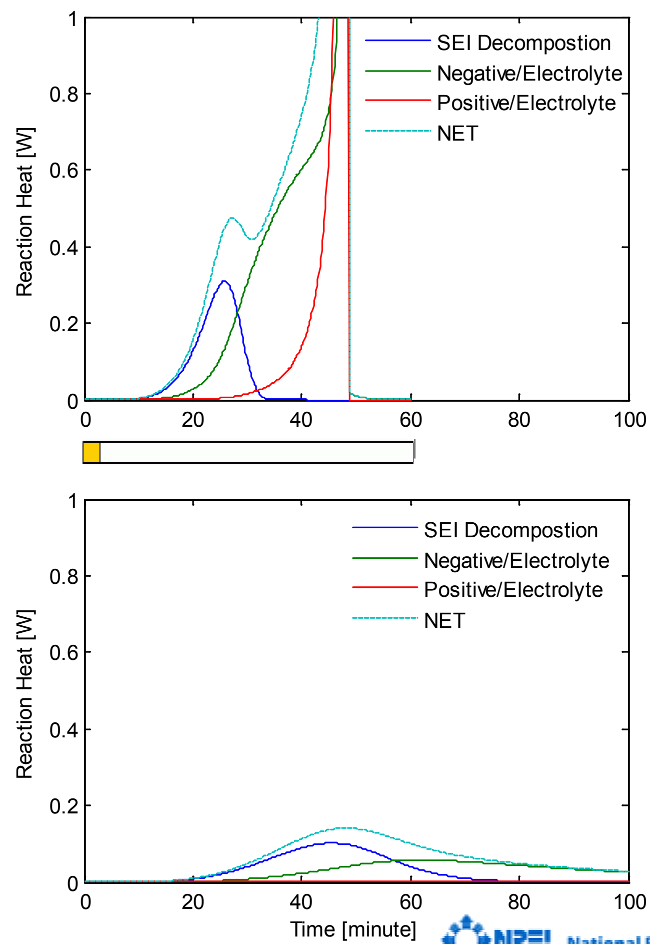
Comparison of Thermal Behavior
Between two High-Resistance Short Events

Temperature



18650 CoO_2/graphite Cell
30°C ambient, (h) = 7 W/m^2K

Component Reaction Heat



7Ω Short
Led to thermal runaway.

Can a short have such a high resistance?

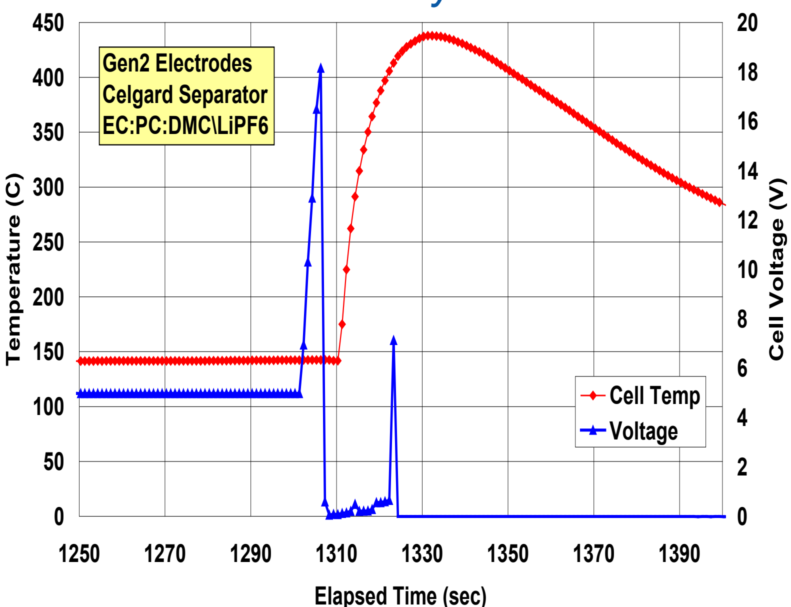
10Ω Short
Did not lead to thermal runaway.

Observed Events

Internal Short (may or may not lead to thermal runaway)

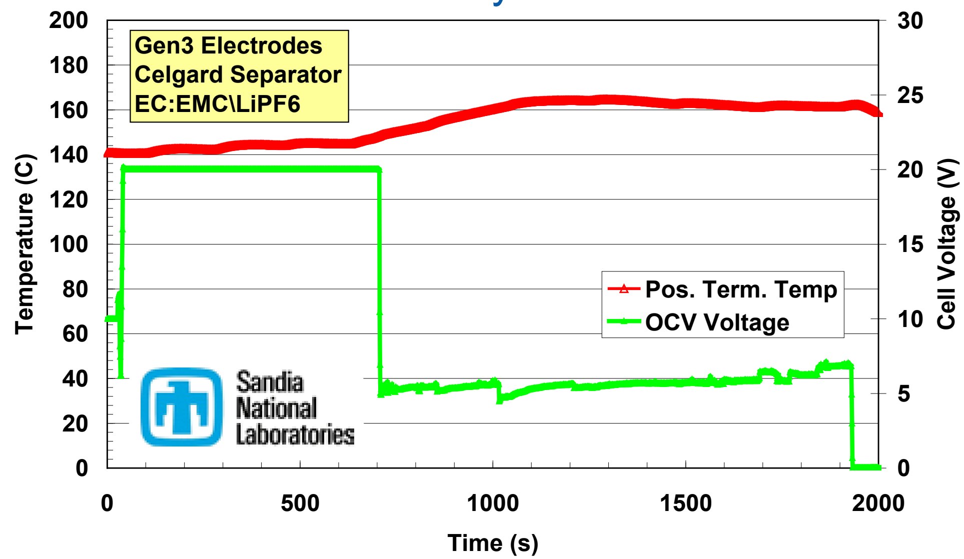
18650 Cells

Short & Thermal Runaway
observed by SNL



- Heat release was much faster than dissipation.
- ***Low resistance short*** (<<1Ω) is likely

- Short occurred at about 700 sec.
- Temperature started to increase and reached thermal equilibrium at about 160°C.
- Thermal runaway was not observed.



- Heat dissipation appears fast enough.
- ***High resistance short*** (>5Ω) is likely.

SNL Data: From presentations at DOE's Advanced Technology Development Meetings
(E. Peter Roth and Tom Wunsch)

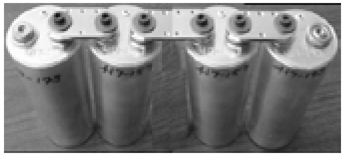
Module-Level Analysis of Cell-to-Cell Thermal Runaway Propagation

How can a module be more resistive to cell-to-cell thermal runaway propagation?

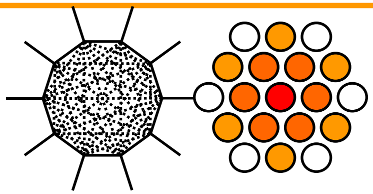
Background

We proposed that *Cell-to-Cell Propagation* in a module is

a result of the **INTERACTION** between the distributed chemical sources and the thermal transport network through a module.



dispersed sources



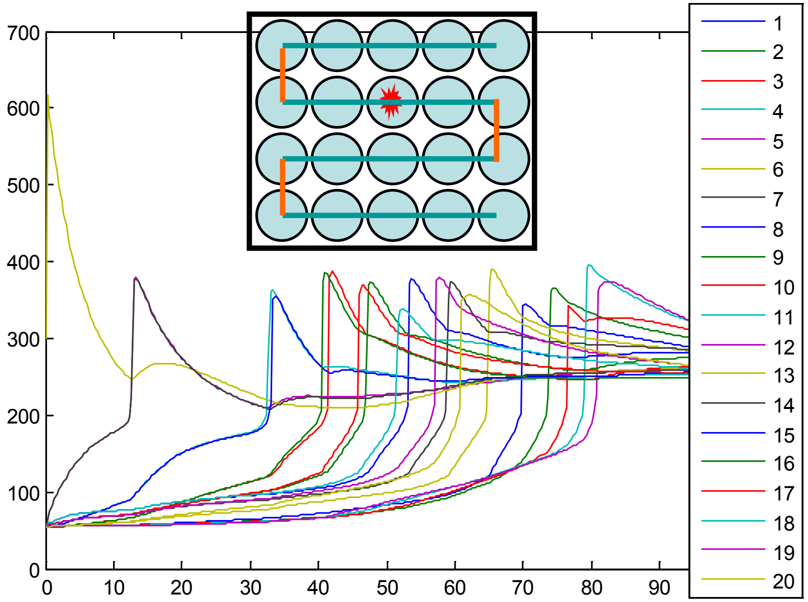
thermal network

Approach *for the analysis of this system*

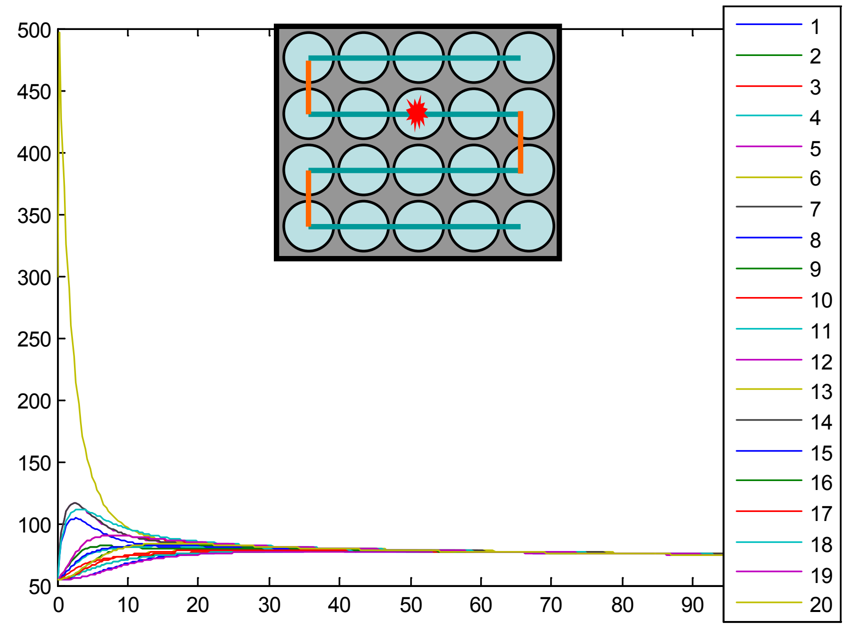
- Formulated *exothermic chemical reactions* of a cell at elevated temperatures.
- Quantified *heat transfer among the cells* in a module
  - → Radiation heat transfer
  - → Conduction heat transfer
  - → Convection heat transfer
- We used multi-node lumped approach last year; this year we have looked at 3D approach

Impact of a Highly Conductive Heat Transfer Medium

Rather than the air used in the base case (left), a highly conductive PCM/graphite matrix was used to fill the space between the cells in the module (right).



Base case (air)



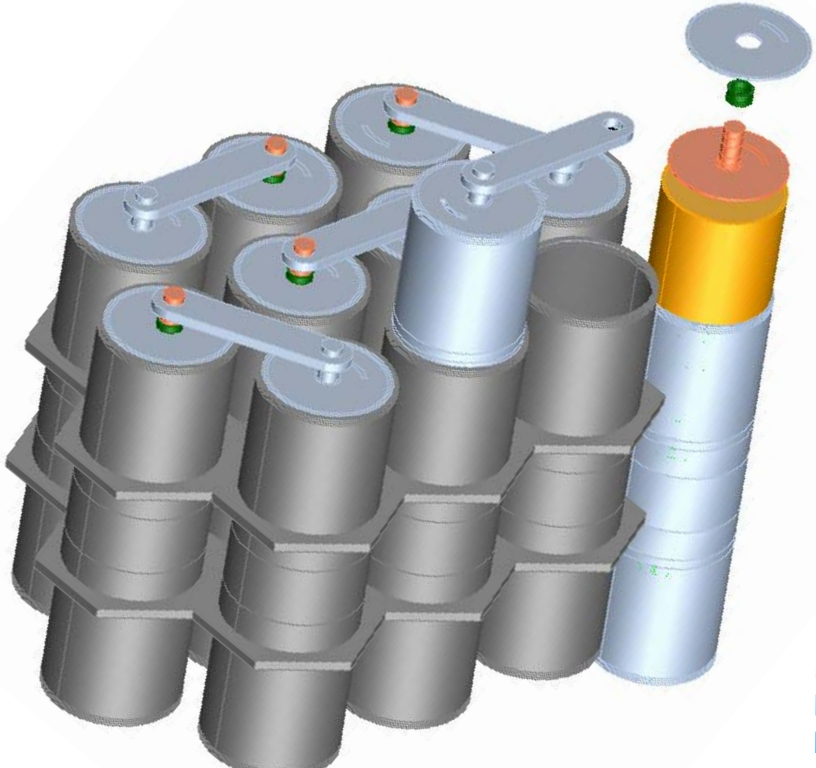
Graphite matrix impregnated with PCM

It appears that a very conductive medium may reduce the chance for propagation.

NOTE: * PCM/graphite matrix is a highly porous graphite structure that is impregnated with phase-change material (PCM) (based on information from S. Al-Halaj et al.).

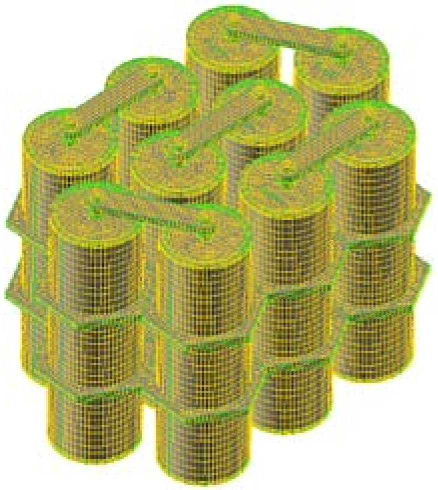
3D Module Propagation Model

Objective: Developing a 3D cell and module geometry capturing cell-to-cell interconnects

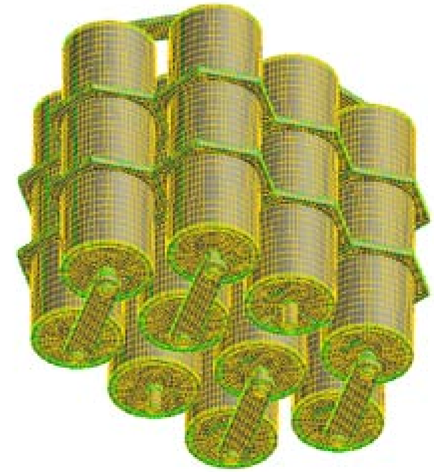


CAD drawing of a 10-cell module
(Each cell is in its own individual sleeve)

Top view

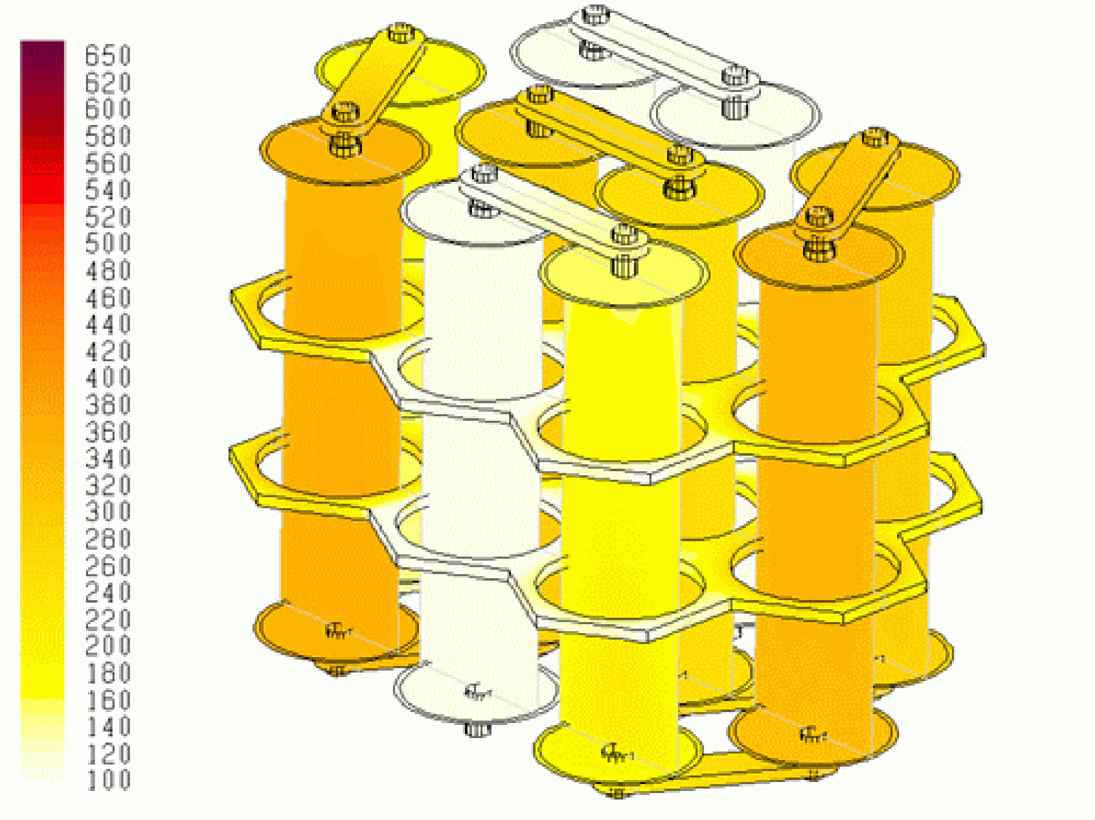


Bottom view



Grid for the 10-cell module

Close Look at Reaction in an Individual Cell in the 10-cell Module



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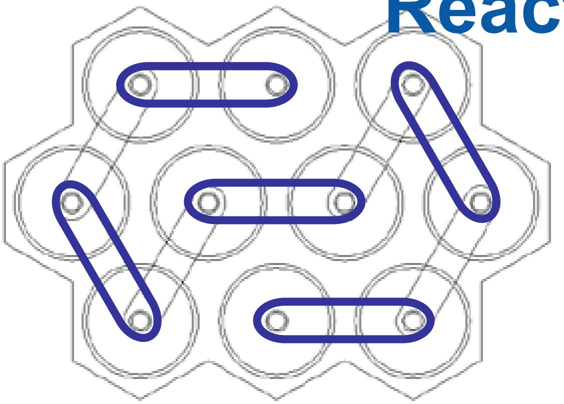
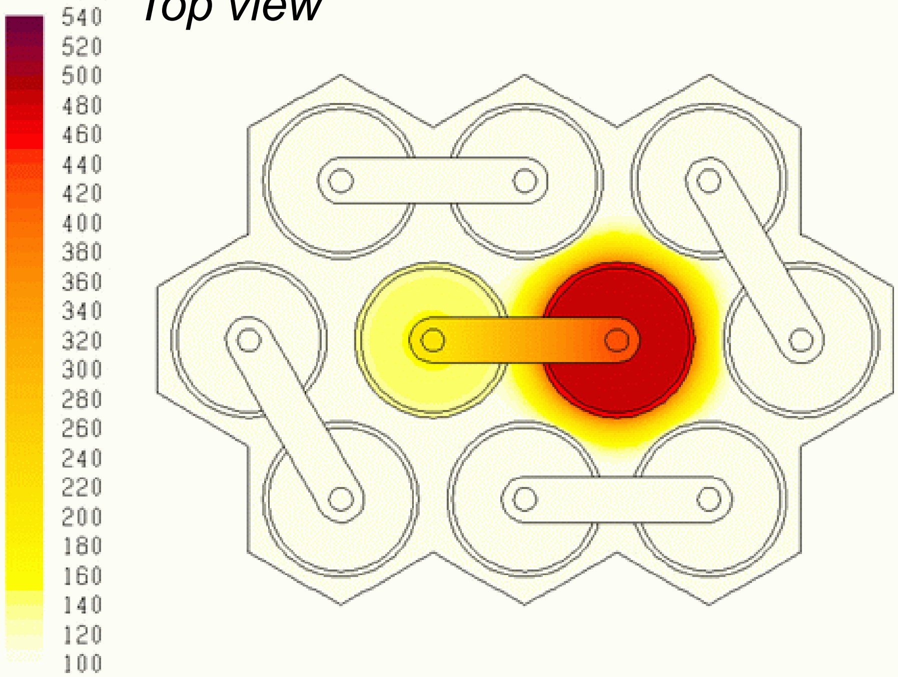
Reaction Propagation in a Module with 10 Cells in Series

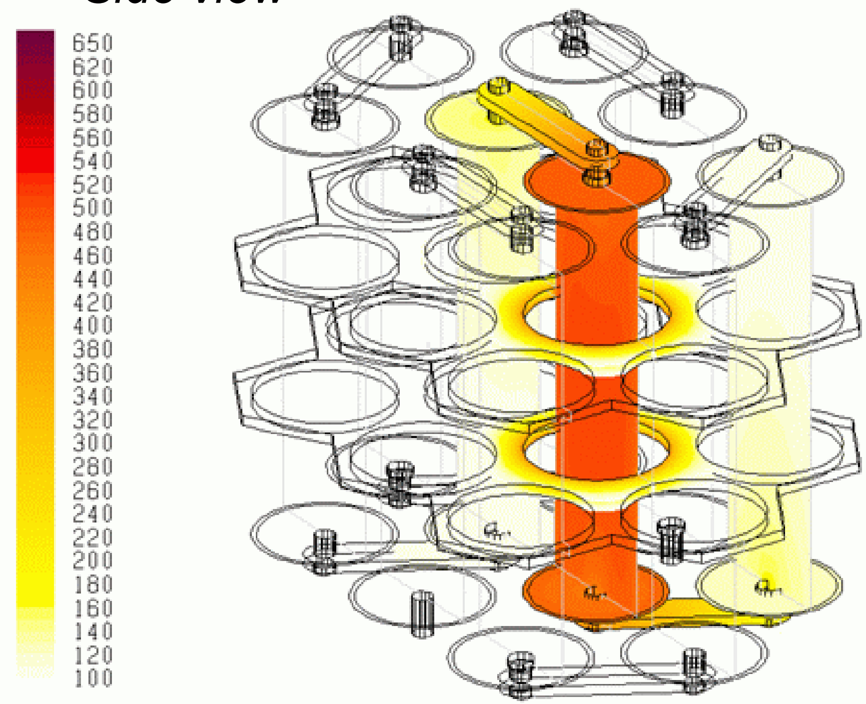


The order at which cells go into thermal runaway depends on the cell interconnect configurations.

Top view



Side view



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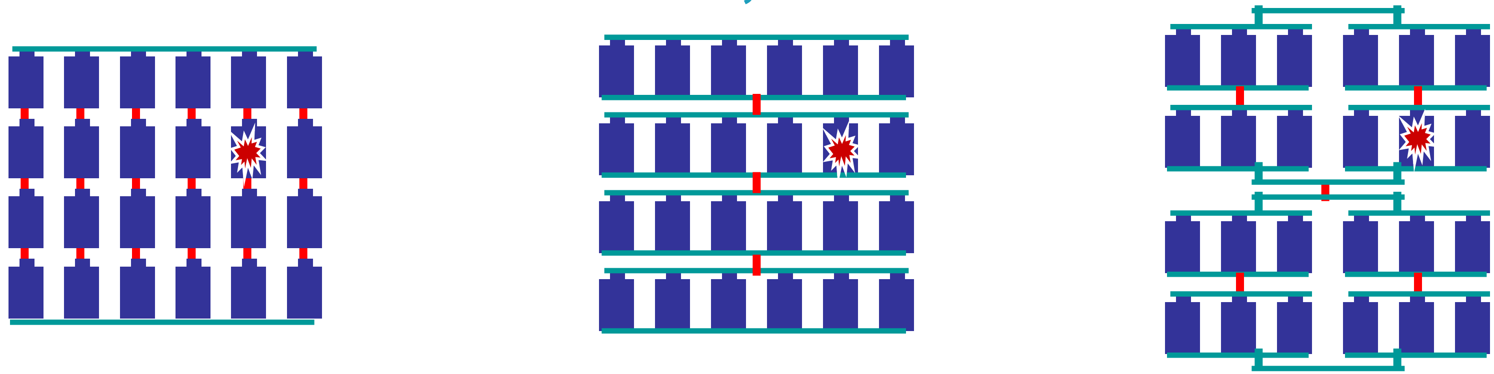
On-going Work
Module-Level Research in Progress

Adding the electrical network modeling

- Impact of thermal transport network + electrical network

6 Parallel, 4 Series



Summary

- Li-ion thermal abuse reaction chemistry was implemented in a finite-volume 3D cell model to address various design elements.
  - ✓ Examined impact of cell design parameters
  - ✓ Investigated impact of short location and thermal properties
    - ✓ Some shorts may not lead to thermal runaway
    - ✓ Heat dissipation is important, but depending on the amount of heat release from abuse
- Propagation of abuse reaction through a module was simulated.
  - ✓ A complicated balance between the heat transfer network and dispersed chemical sources
  - ✓ Balance is affected by module design parameters such as cell size, configuration and size of cell-to-cell connectors, and cell-to-cell heat transfer medium

Future Work

- Improve model through comparisons with *experimental data* from other laboratories
- Continue examining the impact of design variables
- Address the limitation of the model
- Expand the model capability to address *various chemistries* and materials, such as iron phosphate
- Investigate *internal/external short* by incorporating an *thermally coupled electrochemistry model* into the three-dimensional cell model
- Use the models to investigate the impact of (shut-down) separators
- Work with developers on specific cell and module designs

Acknowledgments

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- Tien Duong
- Dave Howell