Lithium Ion Battery Thermal Propagation Modeling: Considerations and Lessons Learned

Dr. Bruce Drolen

Senior Technical Fellow

The Boeing Company

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Short Course Overview

- What is covered here?
 - Why should I care if a Lithium Ion Battery (LIB) experiences thermal runaway?
 - How hot might a failed cell get?
 - What happens when a Lithium ion cell experiences thermal runaway (layman's terms)?
 - How much energy really releases?
 - What are the important heat transfer paths to consider/model?
 - What unique properties should be used?
 - Anisotropic thermal conductivity
 - Specific heat
 - Contact coefficients
 - How much gas releases from a cell during thermal runaway?
 - Useful considerations when correlating thermal runaway/propagation models
- What isn't covered here?
 - LIB electrochemistry and thermal modeling is already covered in an excellent NESC class¹
 - Test results are well covered elsewhere for many different cells and batteries^{2,3,4}
 - Other details are included in a recent paper by a NASA/academia/industry team⁵

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Why should I care if a LIB experiences thermal runaway?



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How hot might a failed cell get? Just look at the spec sheet

- Li-Ion cells have high energy density
 - Substantial system benefits from reduced power storage mass
 - About 4x Ni-Cd and about 2x Ni-H₂
- High energy density presents thermal challenges if a cell fails
- To get in the ballpark, a typical 18650 LIB cell has a nominal capacity of 2.6 Ah at a nominal voltage of 3.7 V and a cell weight of 47 grams; This yields the following
 - Energy = 2.6 Ah x 3.7V x 3600s/hr = 34.6 kJ
 - Cell Thermal Mass
 - 47 g x 0.823 J/g-

	Material	Specific Heat
С		J/g-C
	AI	0.95
	Cu	0.38
	SST	0.50

If electrical energy shorts internally, cell's temperature rise is sudden and large

∆T ~ 34,600 / (47 x 0.823) = <mark>894°C</mark>

- Heat loss paths reduce this temperature rise but not substantially
- Exothermic heat adds to the problem

What happens when a Lithium ion cell experiences thermal runaway (in layman's terms)?

Basic Causes for Propagation of Event

- Adjacent cell fails and heats the neighbor's case and windings
- Separator material b/w anode & cathode layers melts or at least softens to allow contact between electrodes
- Electrical short occurs between anode and cathode across separator

Sources of available energy

• Stored electrical and exothermic chemical energy

Energy release mechanism

- Stored electrical energy heats cell as windings come in contact
- Release is quick, almost all energy goes to warming of cell's thermal mass
- Chemical reactions ensue as cell warms above given thresholds

Venting mechanism

- As cell temperature increases the electrolyte vapor pressure increases
- Internal pressure exceeds max pressure of vent port
- Vented gas carries significant energy away from cell that can heat other cells or other hardware/electronics in the pack

How much energy really releases during a runaway event?

- It is overly simplistic to assume that all the electrical energy releases during the rapid short within the cell that occurs during thermal runaway
- An existing NESC lesson¹ showed that the amount of energy released and the efficiency of that release is greater for low C-rates
 - the higher the C-Rate the less electrical energy can be released
 - It is a rate chemistry thing
- The electrical energy that releases drives the cell hot very quickly
 - Results in exothermic reactions fed by both the cathode material and the electrolyte
- Calorimetric tests have been done on many cells to measure the energy released during thermal runaway⁷
 - the total energy release is about 1.4 X the rated energy of the cell, to within about 15%

What are the important heat transfer paths to consider/model?

- Somewhat Obvious:
 - Model the structure of the enclosure and the hardware holding the cells in place
 - This is relatively straightforward kA/L and mC_p kind of work that we do every day
 - My advice is to use finite difference and lumped parameter type of modeling (TD for instance) so it is easy to pin node numbers to key surfaces and features in the model for logic and parameterization purposes
 - During Thermal Runaway (TR) events there can be large temperature gradients so try not to use too coarse of a model
 - The box and associated structure might want to be nodalized at least at the level of cell dimensions and probably a good bit finer

What are the important heat transfer paths to consider/model?

- Not so obvious:
 - The core of the cell is a winding, often called a "jelly roll" that is made up of a roll of anode/separator/cathode layers somewhat like a toilet paper roll
 - The conductivity along the axis is far better than it is radially
 - You need greater resolution in the radial direction than in the axial direction
 - Temperatures during TR events can be very high; this can make radiation an important heat transfer path
 - Glue lines between cells and other such paths that are thermally unimportant during normal operation can be critical during TR events
 - Many of the dimensions between cells are so small that natural convection is suppressed and the air surrounding the cells can best be treated as another conduction path
 - When a cell vents, significant gas is released which, depending how the pack is vented, may force the addition of forced convection terms in the model
 - Cell mass often changes significantly during a TR event so the thermal mass of the cell will need to be adjusted when the event is triggered in the model
 - Contact coefficients such as winding-to-cell-can and can-to-structure can be key choke points. Parameterize these in your models to allow easier correlation of models to test

What unique properties should be used?

- Anisotropic thermal conductivity
 - Thermal conductivity along the length of the cell is far higher than that across the layers of the winding
 - Can be estimated based on the constituents of the cell and intimate thermal contact between layers
 - Good contact is supported for cell wetted with electrolyte prior to runaway event
 - Reasonable estimate: k_{long} = 30 W/m-K, k_{rad} = 0.2 W/m-K
 - Measured values for 18650 cells as reported by Drake, et al.⁸

Specific heat

- Measured values indicate that a specific heat somewhat less than that of aluminum is appropriate
- Roth⁹ reported measured values of 0.82 to 0.9 kJ/kg-C for two different commercial 18650 cells
- 0.83 kJ/kg-C has been reported for the specific heat of the jelly roll within the cell
 - As used by Coman, et al.¹⁰ referencing measurements by Richard and Dahn¹¹

Contact coefficients

- Prof. Amy Marconnet and her team measured the contact heat transfer coefficient between the separator surrounding the cell winding and the cell can wall (measurements were made dry)¹²
- The mean measured interface conductance was 670 W/m²-K with a standard deviation of 275 W/m²-K

How much gas releases during thermal runaway?

Vented Gas Volume per Roth and Orendorff¹³



5 different Lithium ion chemistries yielded the same gas volume per Ah at end of venting, 1800 mL STP/Ah

FIG. 4. Normalized ARC gas generation profiles from 18650 cells of several cathode chemistries showing equal gas volumes per Ah generated at end of thermal runaway.

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Useful considerations when correlating thermal runaway/propagation models

- Thermal runaway tests are often initiated with a warm-up of the pack and or the trigger cell
- This may be the most controlled portion of the test
 - Known heat loads (heaters)
 - Geometry is pristine (cell and/or structure hasn't deformed yet)
 - Surfaces are clean (no soot yet)
 - Mass of cell is known
 - No forced convection in the battery box
 - Temperatures are relatively low so radiation not as significant
- If the model doesn't track the test data prior to the TR event your chances of reaching good correlation FOR THE RIGHT REASON during and after the TR event are minimal
- Be prepared to change terms in your model during and after the TR event to reflect loss of cell mass, accumulation of cell ejecta giving conduction paths that did not exist in the pristine pack, and other geometry changes

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