Distributed Heat Load Approach to Thermal Runaway Simulation

Bridging the Gap Between Simulation and Reality

Dr. William Q. Walker
Research Scientist I

with contributions and collaborations from:

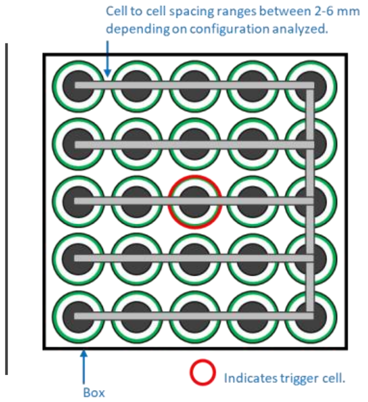
Tapesh Joshi, Ph.D. & Judy Jeevarajan, Ph.D.

The Electrochemical Safety Research Institute (ESRI)
Underwriters Laboratories

BACKGROUND

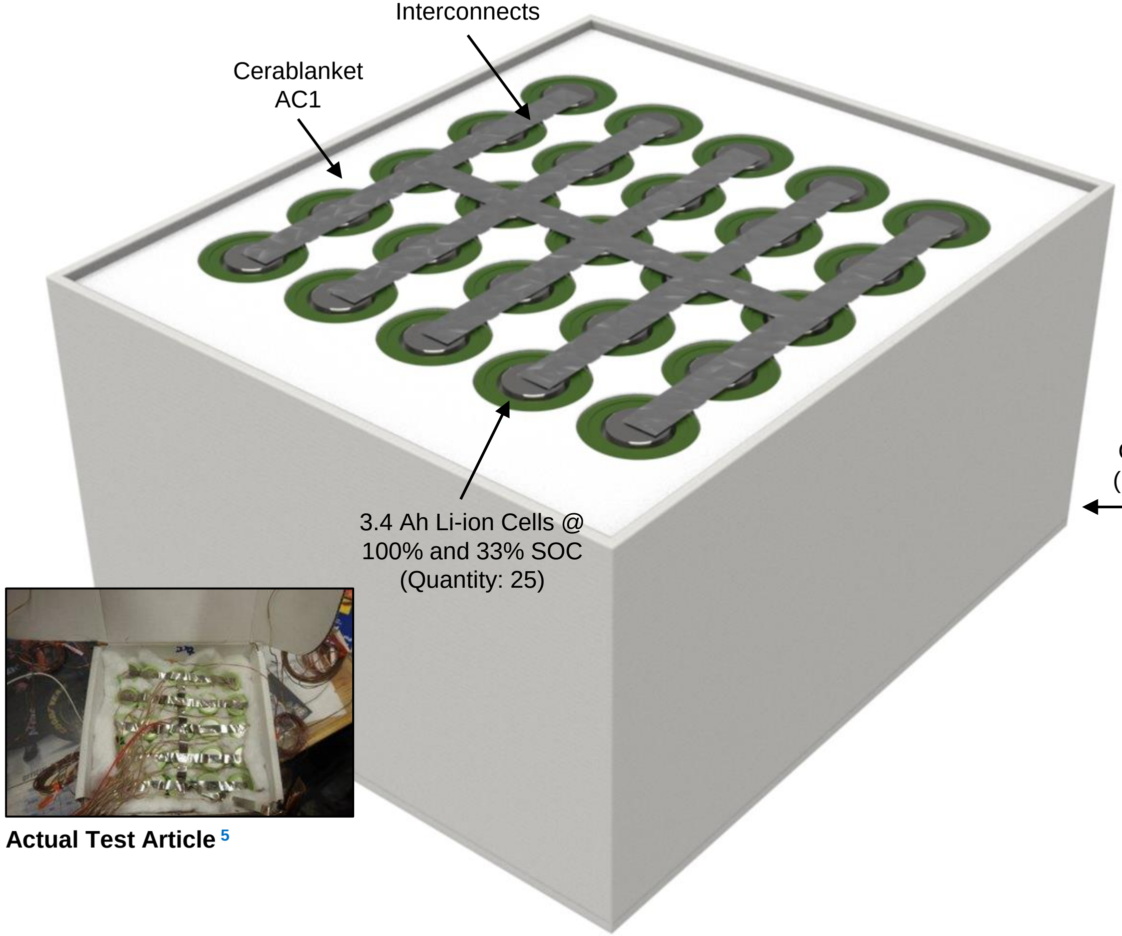
- **Underwriters Laboratories has been conducting Li-ion battery thermal runaway abuse testing to evaluate the protection offered by various insulation types of varying thermal properties:**
  - Test articles have been in the form of transportation boxes as depicted with the images below.
  - 25-Parallel (25P) 3.4 Ah 18650 format cells with 2-6mm spacing. [5]
  - 100% and 33% SOC. [5]
  - Central trigger cell with 10 °C min^{-1} heating rate. [5]
- **These past experiments serve as the focal point for this analytic case study.**
- **Detailed Thermal Desktop® models of the test articles were developed and used to further analyze the thermal response of the test articles:**
  - Rather than a multi-physics approach, these models rely on user defined heat loads coupled with a detailed conduction and radiation models.
  - Final model correlation activities are still underway, so the presentation today will focus on the general technique, approach, and utilization of the models to simulate specific user defined thermal runaway conditions.
  - For time management, results presented reflect the **Configuration A 100% SOC test article**, but results for the other configurations and SOCs will be made available in the back-up section of the posted presentation.

Images courtesy of Jeevarajan, Joshi, & Lenoir [5].

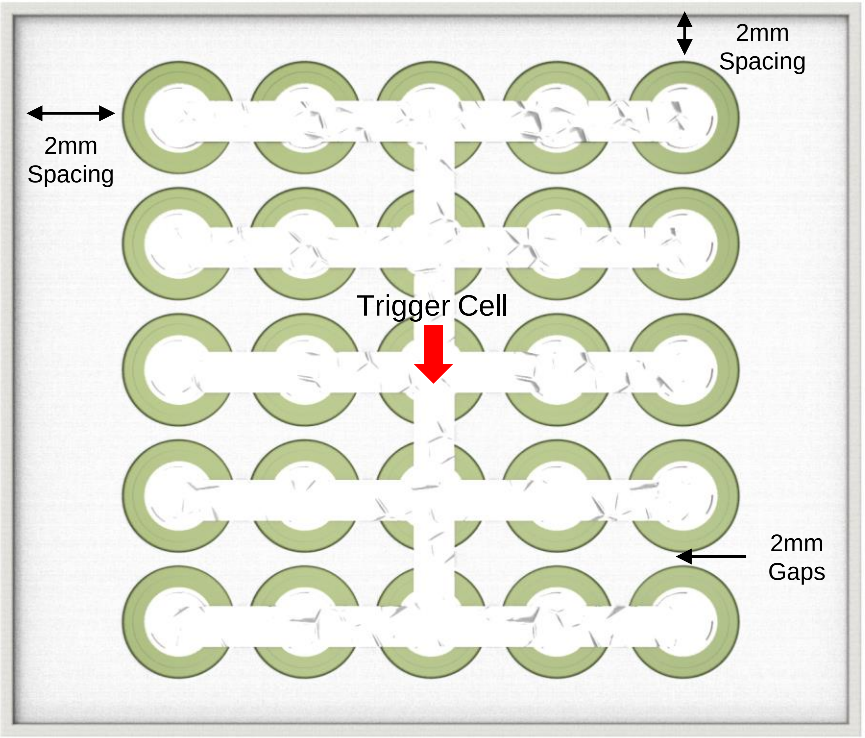


[5] Jeevarajan, Joshi & Lenoir, “Mitigation Methods for Fire and Thermal Runaway Propagation in Li-ion Modules”, International Battery Seminar and Exhibit (2021).

TEST ARTICLE DESCRIPTION

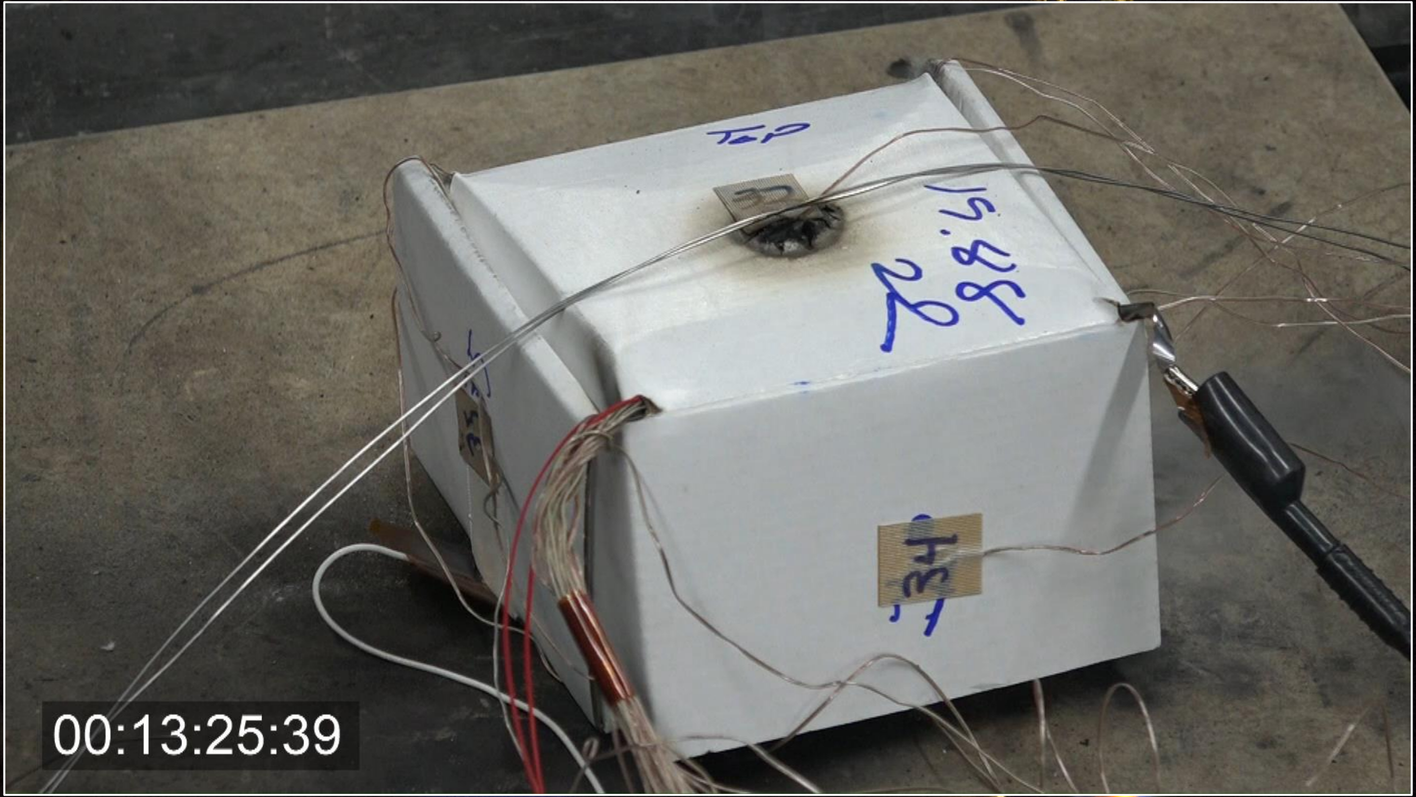


Actual Test Article [5]



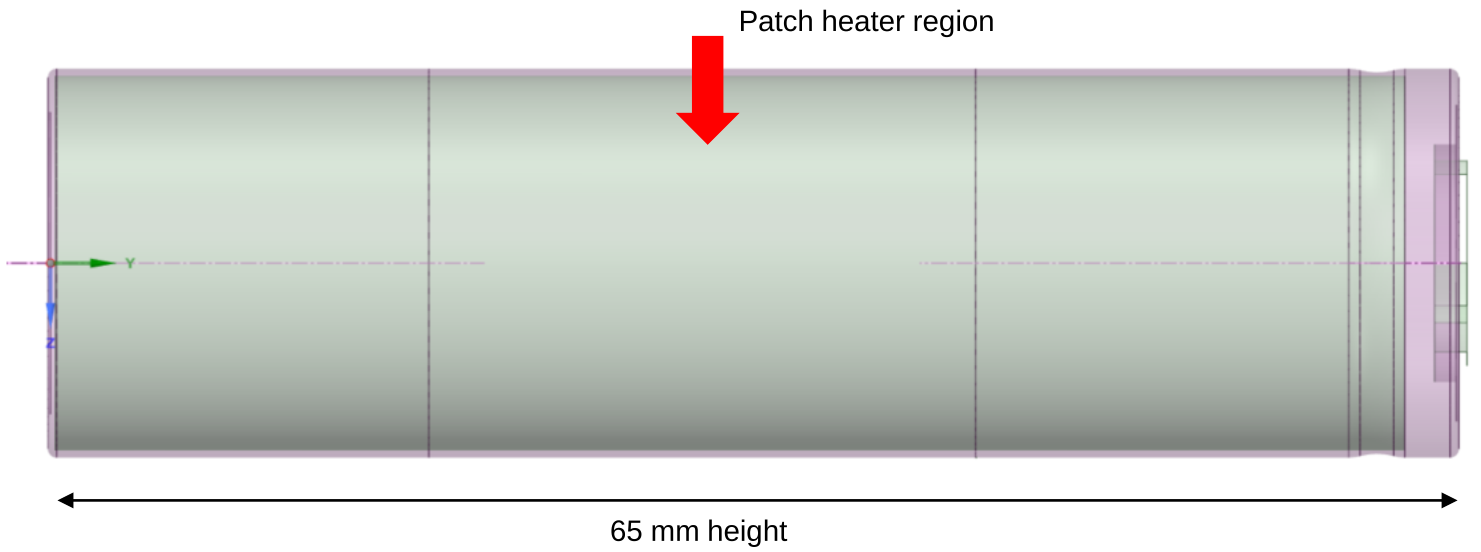
[5] Jeevarajan, Joshi & Lenoir, "Mitigation Methods for Fire and Thermal Runaway Propagation in Li-ion Modules", International Battery Seminar and Exhibit (2021).

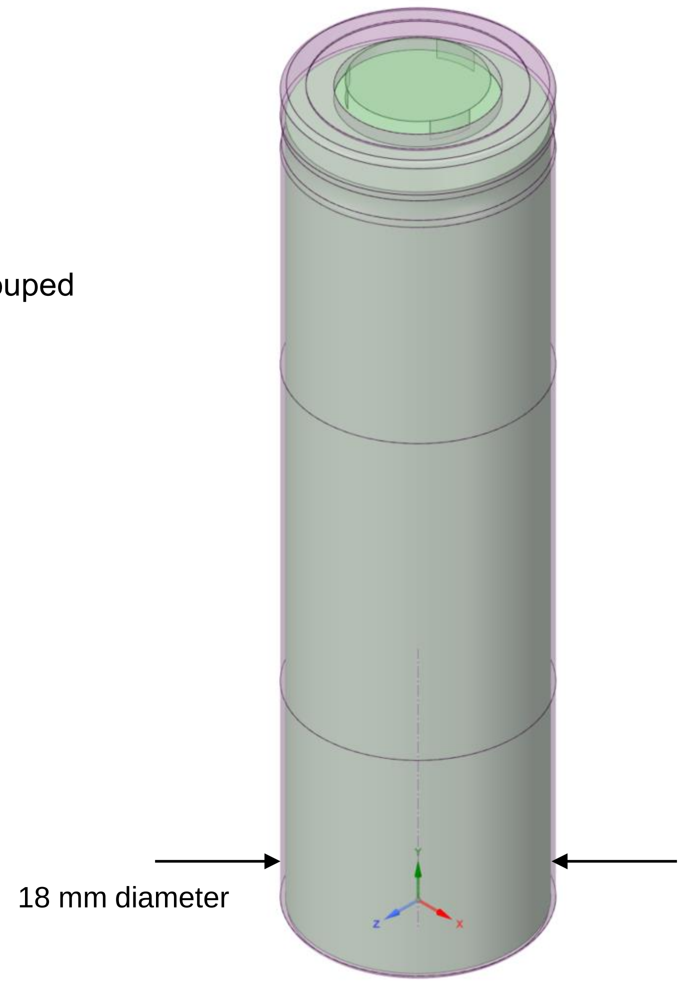
For perspective, take a quick look at what we are trying to simulate.



MODEL DESCRIPTION

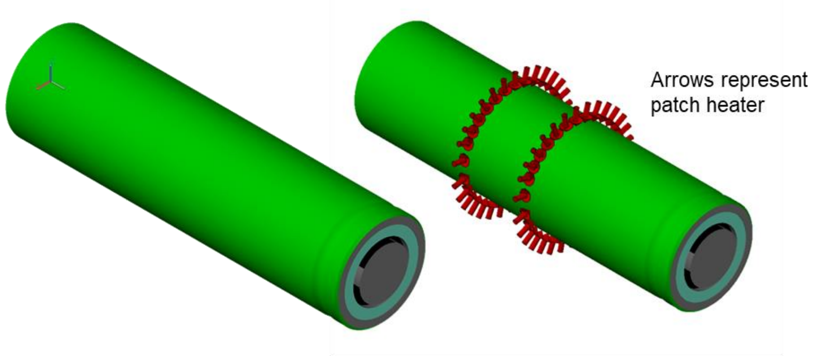
- **First step was to develop CAD of an 18650 cell that could serve as a repeated use reference, or child, model and to prepare it for thermal modeling activities.**
- **CAD of 18650 prepared for thermal modeling in ANSYS SpaceClaim®.**
- **Included distinct representation of the cell casing vs. electrode winding:**
  - Casing geometry represented with surfaces (transparent in images).
  - Electrode winding geometry represented with single cylindrical solid (non-transparent in images).
  - The central 2" region of the cell casing where the patch heater was applied during testing was specially grouped for later access in the thermal model.





MODEL DESCRIPTION

- **ANSYS SpaceClaim® geometries of the general 18650 cell are linked to Thermal Desktop® using TD Direct®.**
- **Via TD Direct® the following are managed:**
  - Assignment of material properties (thermophysical and optical).
  - Creation of Domain Tag sets to be used to access surfaces and solids of interest (contactors, heat loads, et…).
  - Assignment of meshing controls.
  - Simultaneous meshing and import into Thermal Desktop.
  - Final product shown with images below.
- **Cell casing to electrode winding contact resistance of 670 W m^{-2} °C^{-1} based on findings by Gaitonde et. al. [6].**
- **Once in Thermal Desktop®, the child model of the single 18650 cell was imported into another Thermal Desktop® model 25 times using AutoCAD XREF features to create the parent model:**
  - Updates to the SpaceClaim file will automatically synchronize with the child Thermal Desktop® model.
  - Updates to the child Thermal Desktop® model will subsequently be propagated throughout the parent Thermal Desktop® model.



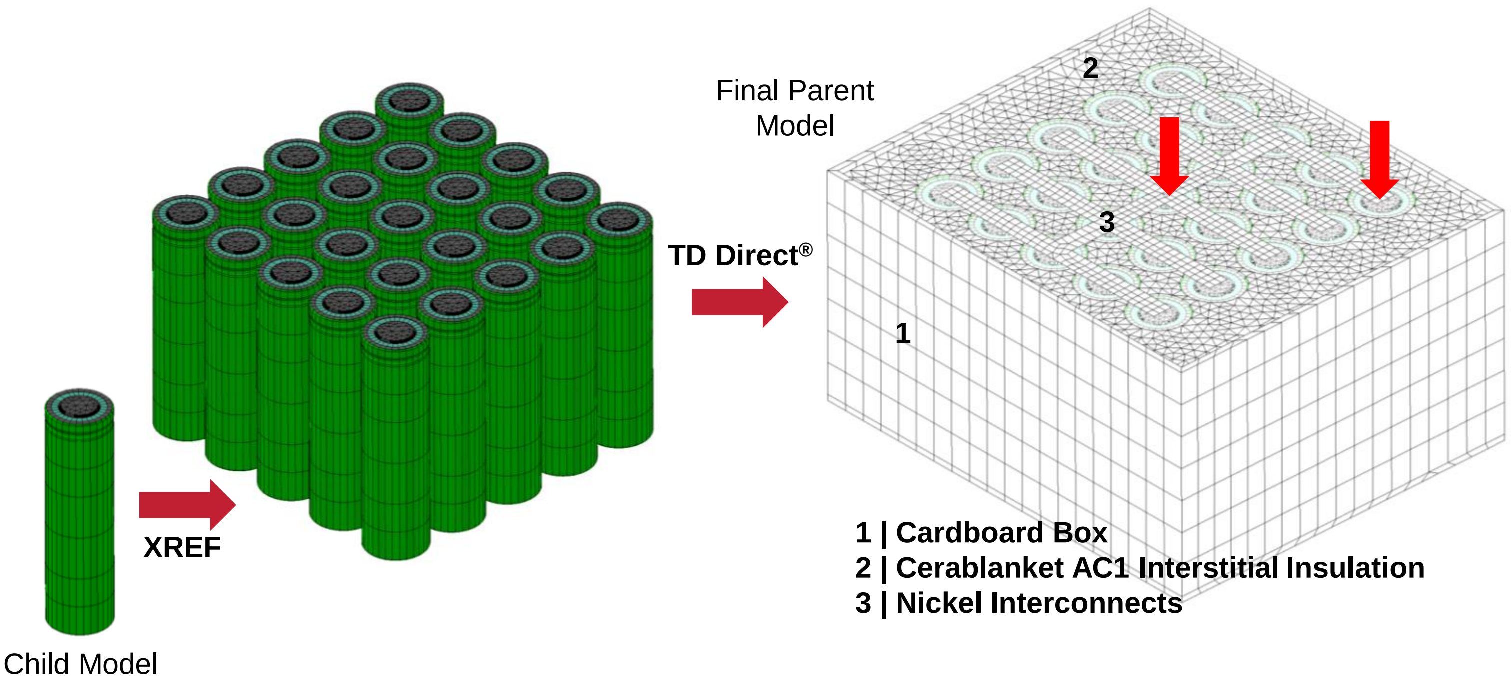
Material	k (W m^{-1} C^{-1})	C_p (J kg^{-1} °C^{-1})	ρ (g cm^{-3})
[7] Steel	45	500	7.85
Electrode Winding	1, 25, 25 (x y z) [8]	1000	2.8
Combined cell casing and electrode winding mass is 47.5 g.			

Very important to represent anisotropic thermal conductivity

[6] Gaitonde et. al., “Measurement of interfacial thermal conductance in lithium ion batteries”, Journal of Power Sources (2017).
[7] NASA Engineering and Safety Center (NESC), “Open Thermal Desktop Properties Database v1.3”, NASA (2016).
[8] Chen, Wan, & Wang, “Thermal analysis of lithium-ion batteries”, Journal of Power Sources (2005).

MODEL DESCRIPTION

- **The primary features of the Configuration A thermal model include the following:**
  - Cerablanket AC1 interstitial in-between the cells and between the cells and the box.
  - Testing conducted with central trigger cell with heating rate of 10 °C min^{-1}; analysis considers both central and corner trigger cells.
  - Currently, analysis assumes 2” circumferential patch heater @ 100 W to reduce the time to trigger *(will refine later)*.
  - 40 kJ cell body thermal runaway heat load released over 2 s to the electrode winding solid elements.
  - Thermal runaway heat is released if any node within the electrode winding exceeds 100 °C.
  - Currently not accounting for ejecta heating *(will be included with next steps of this analysis)*.
  - Negligible interface thermal resistance between contacting surfaces *(will be refined during model correlation activities)*.



Material	k (W m^{-1} C^{-1})	C_p (J kg^{-1} $°C^{-1}$)	ρ (g cm^{-3})
[1] Cardboard	0.5	1400	0.69
[2] Cerablanket AC1	0.08 to 0.54	1130	0.096
[3] Nickel	397.5	384.9	8.94

[1] Determined from general internet search. Should refine later.

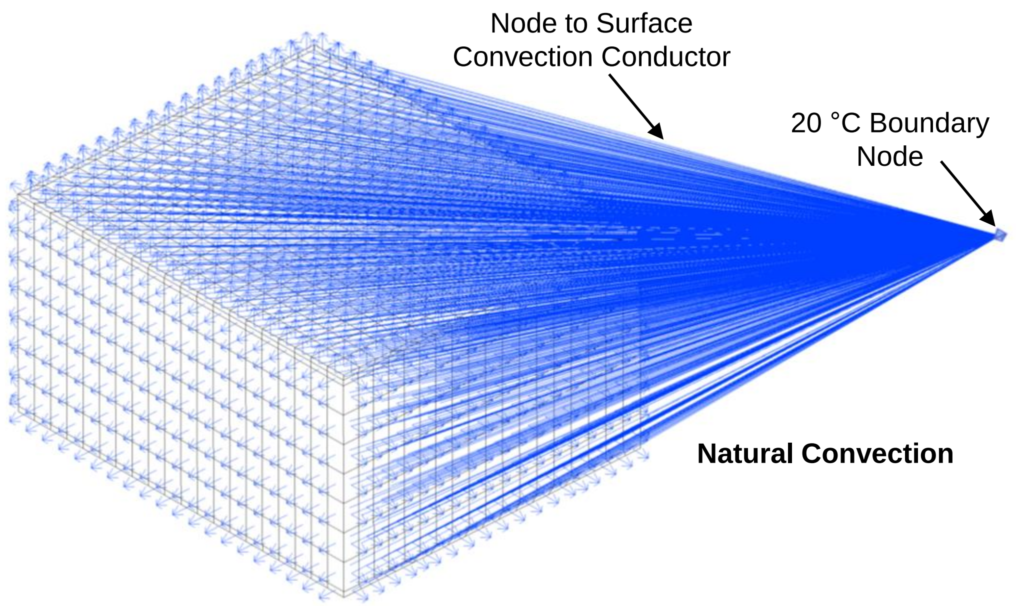
[2] Determined from Morgan Advanced Materials Cerablanket AC1 datasheet on the ESRI team SharePoint and a general Cerablanket datasheet found online.

[3] Determined from the NESC Thermal Desktop Properties Database.

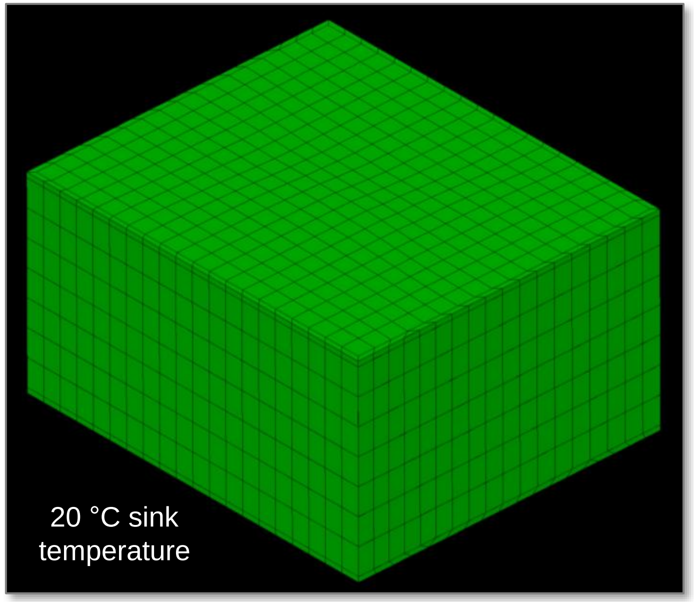
Indicates trigger cells in analysis

ANALYSIS BOUNDARY CONDITIONS

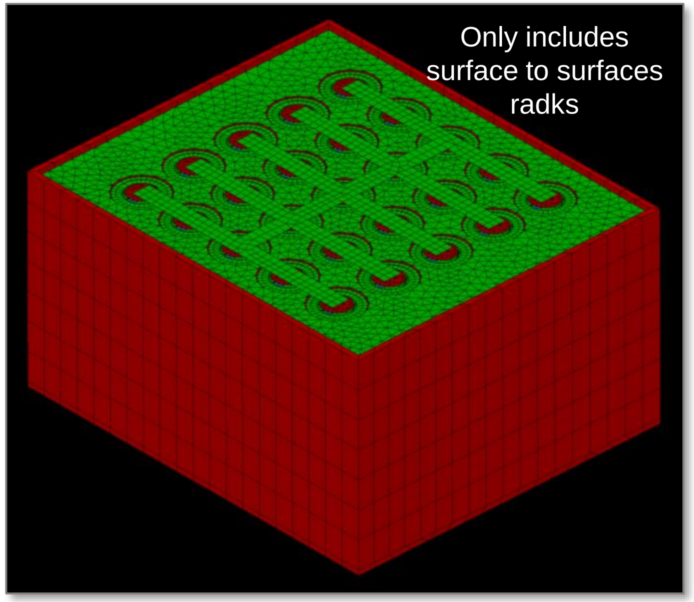
- **Natural convection (h: 5 W m^{-2} $°C^{-1}$) and radiation to a 20 °C sink temperature:**
    - Natural convection is user defined (not auto calculated by Thermal Desktop®).
    - Automatic radiation calculations and user defined natural convection calculations are performed on external surfaces only.
- **Internal surface to surface radiation within box where applicable.**
- **Boundary temperatures and convection conductor are set-up as symbols to support parameterization.**



External Radiation Surfaces

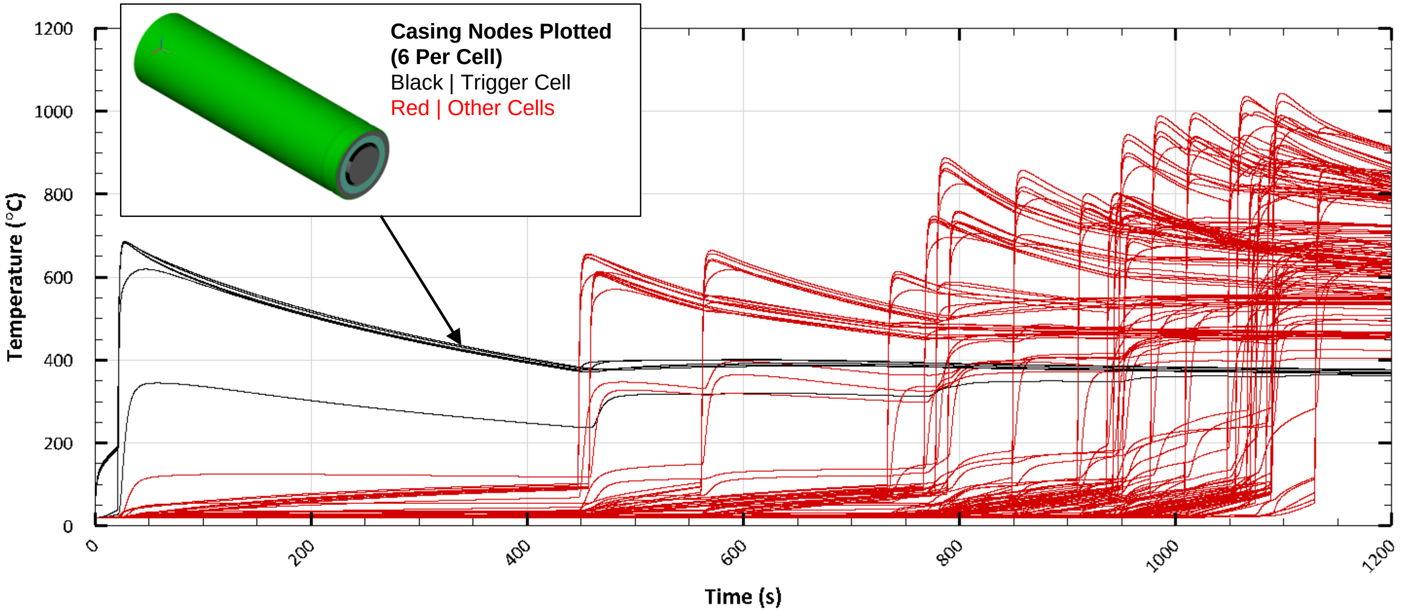


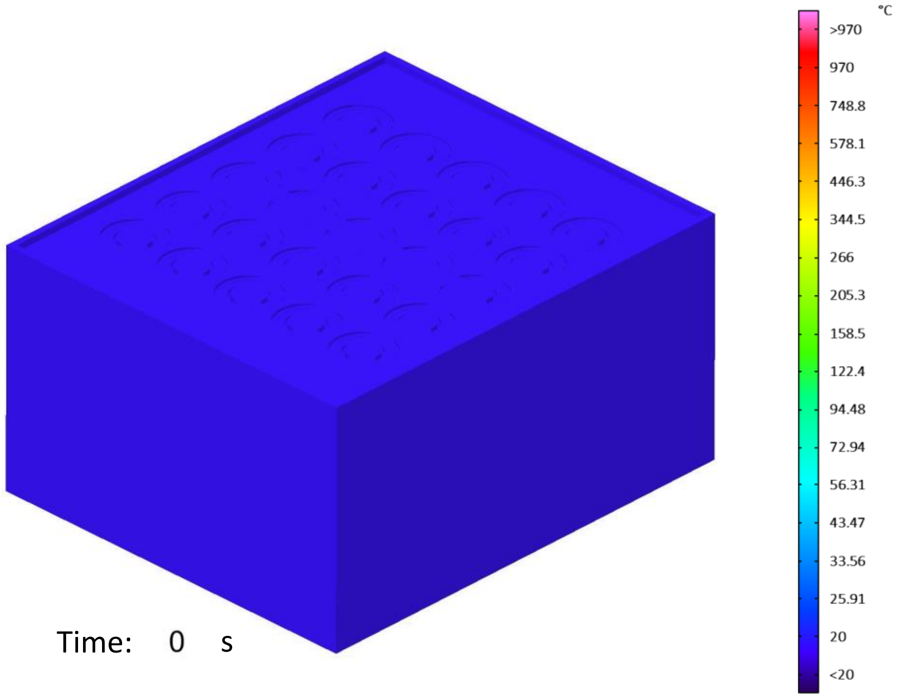
Internal Radiation Surfaces



RESULTS | CORNER TRIGGER

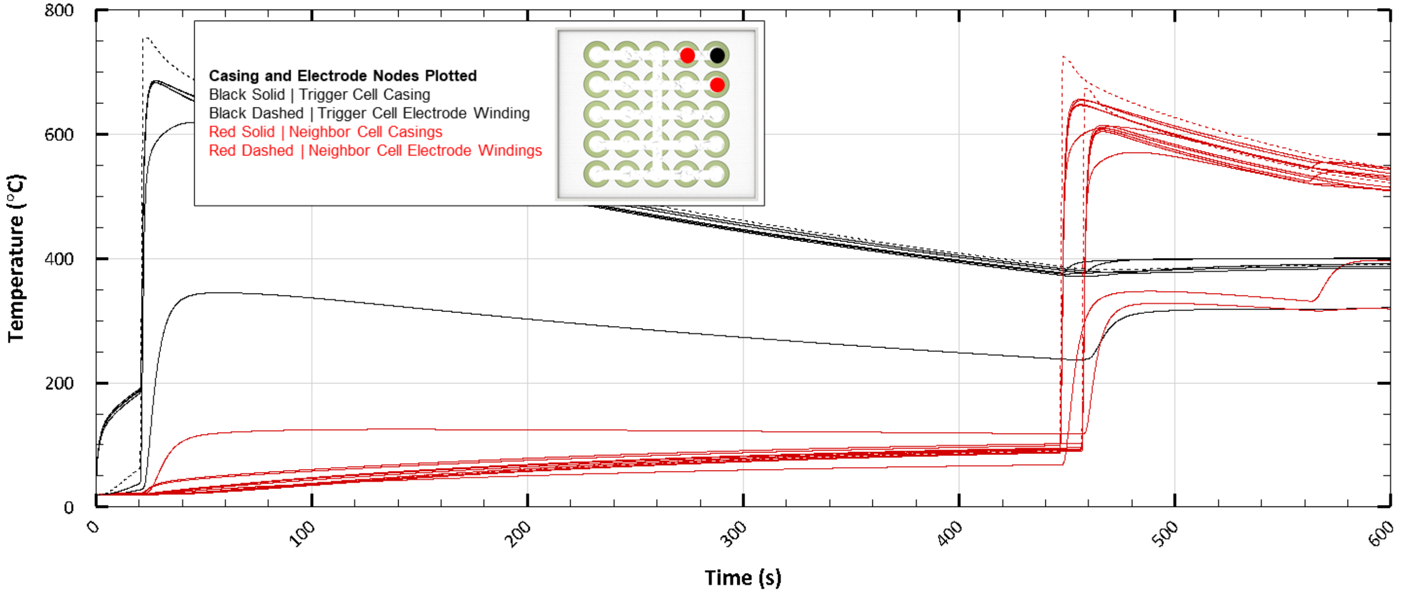
- **Results are shown here for the following conditions:**
  - Corner cell trigger.
  - 90 kJ thermal runaway event with 50% released through cell casing (45 kJ).
- **Thermal simulation indicates that conditions analyzed would likely result in cell-to-cell propagation:**
  - First propagation event would be ~425 seconds following the initial event.
  - Time to next event is significantly reduced with addition of heat from a previous event.
  - Heat from second event induces a rapid chain reaction that would be extremely difficult to stop.

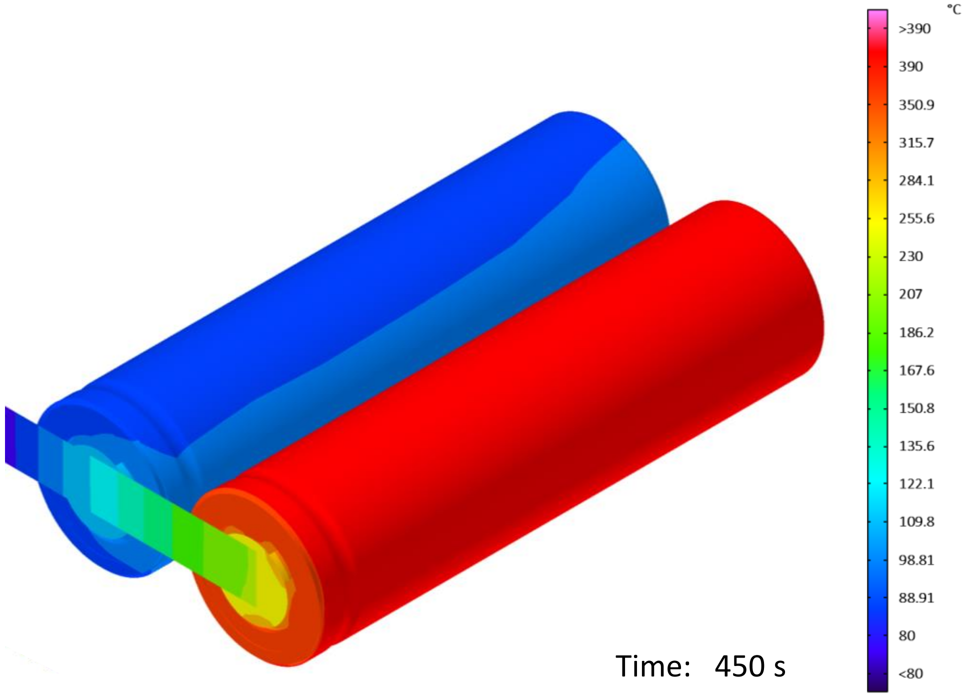




RESULTS | CORNER TRIGGER

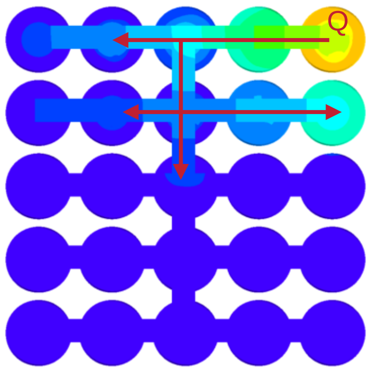
- **Recommend giving consideration to internal temperature profile when evaluating external temperature measurements.**
- **Central nodes from the electrode windings for the corner trigger cell and neighbor cells are plotted (dashed lines) along with the corresponding cell casing nodes (solid lines):**
  - Due to the thermal resistance between surfaces, the electrode winding is warmer than what would be ready via external temperature measurement following thermal runaway.
  - Considerable gradient could exist throughout the cell casing and also between cell casing vs. electrode winding.
  - When evaluating abuse test results vs. success criteria, it is important to not just consider the temperature measured by a thermocouple on the cell casing, but also the temperature achieved by the electrode winding and how long those temperatures may have sustained.



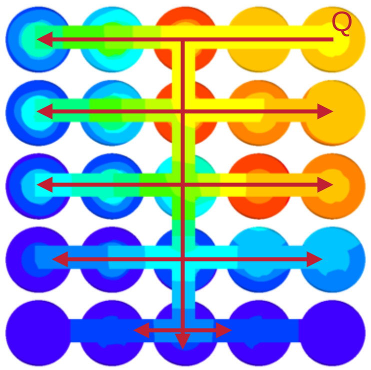


RESULTS | CORNER TRIGGER

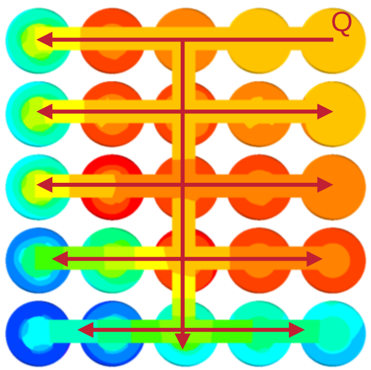
- **The thermal model can also help describe heat movement through the interconnects:**
  - The images and video below help describe the heat movement through the interconnects for the conditions simulated.
  - Note that increasing amounts of cell body heating and low thermal resistance interconnect to cell welds will result in higher amounts of thermal runaway heat transferred to neighboring cells in a short period of time.
- **Depending on the condition and weld type, combined with the heat generated from thermal runaway, the conductive path created by the interconnects can be enough to facilitate cell-to-cell propagation.**
- **This path should always be considered when balancing the need for heat sinking vs. insulation.**
  - The impact of ejecta and associated heat landing on the interconnects should also be consic
  - Said ejecta can also causes external shorting which will also generate heat.



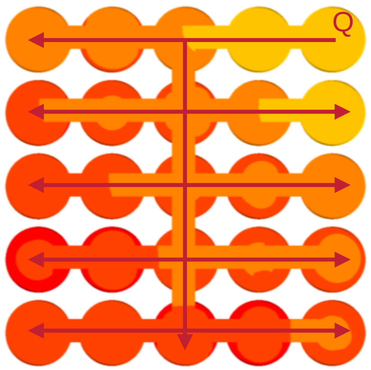
Time: 400 s



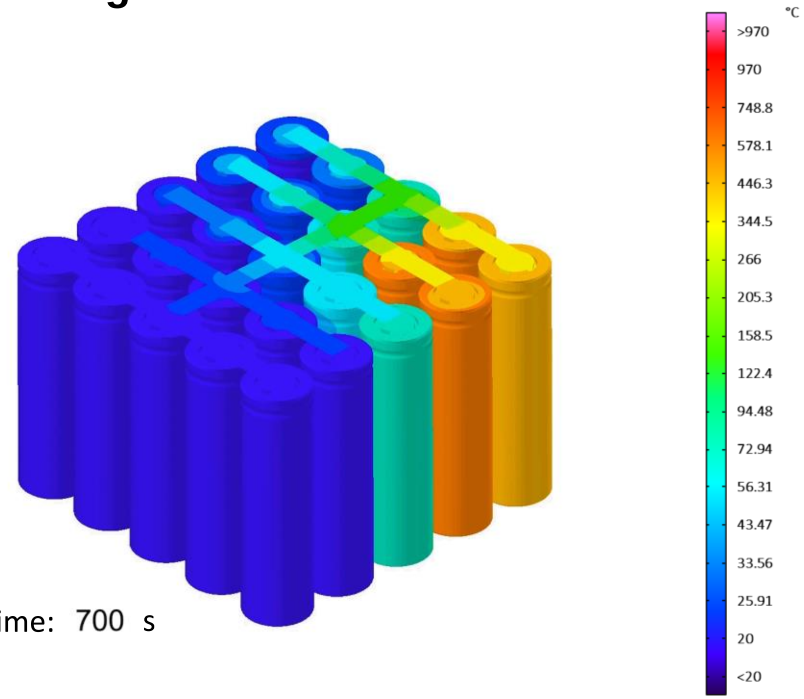
Time: 800 s



Time: 1000 s



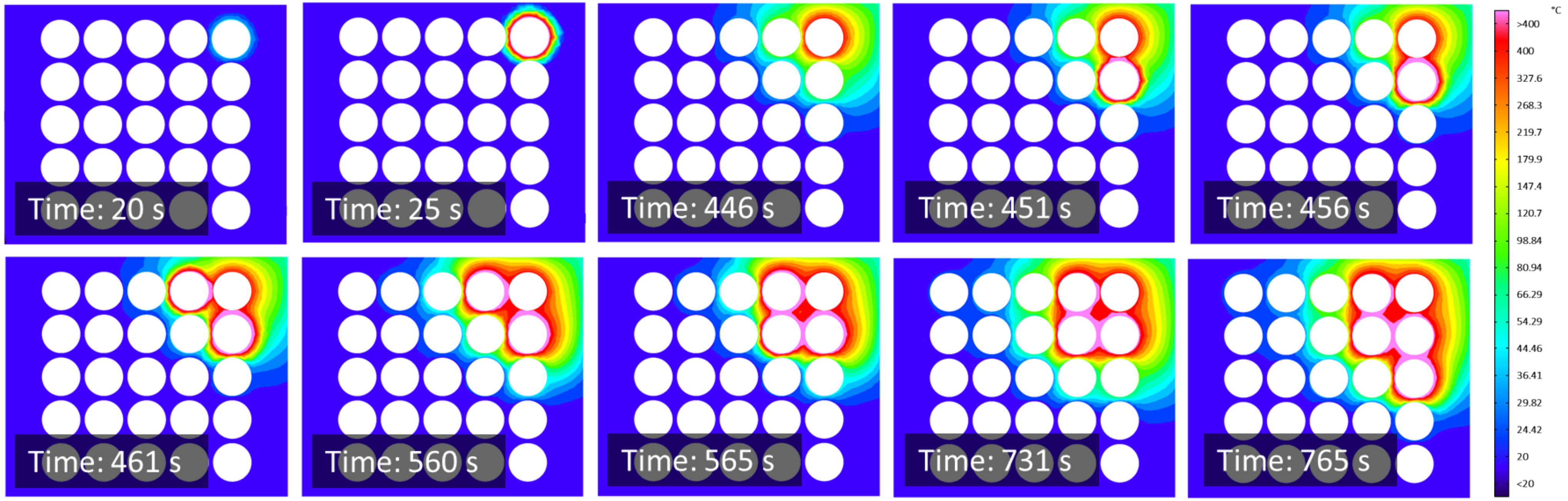
Time: 1200 s



Time: 700 s

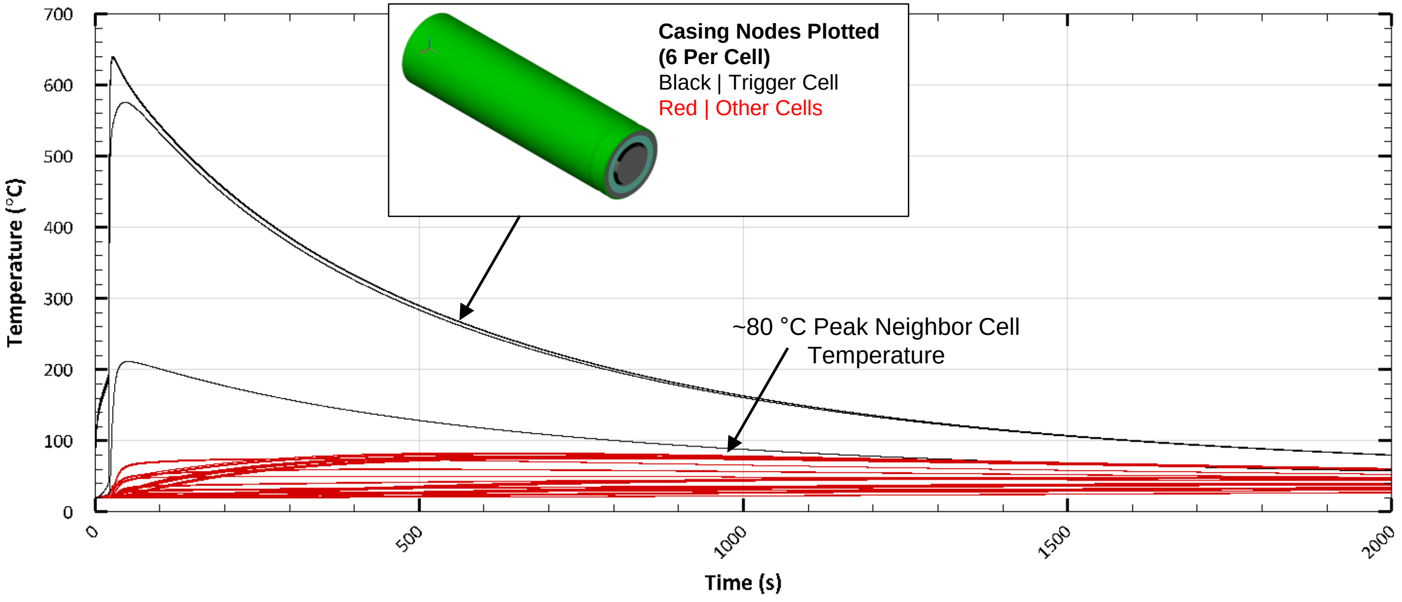
RESULTS | CORNER TRIGGER

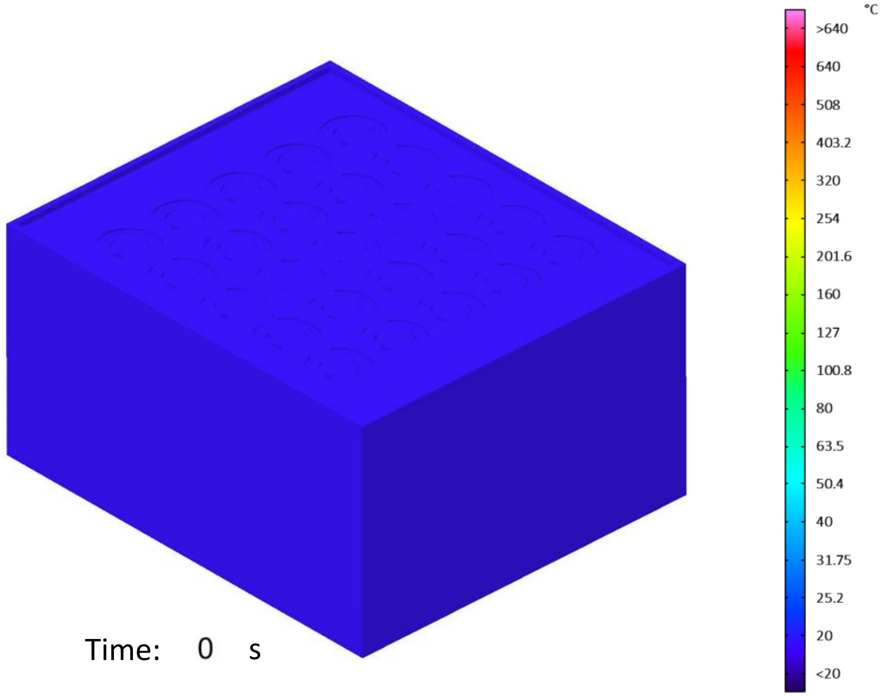
- **Evaluation of the heat transfer strictly through the interstitial insulation, in this case Cerablanket AC1, can also be helpful in understanding how the design might behave.**
- **The Cerablanket AC1 offers strong protection from the initial event, but without heat extraction analysis indicates that the heat will eventually conduct to neighboring cells and initiate cell-to-cell propagation:**
  - Initial event occurs around 20 s with the second event not occurring for another 425 s.
  - After heat of second event is introduced, time between events is drastically reduced.
  - Effective design is a balance between insulation and heat extraction – distributed heat load analysis can help identify this balance.



RESULTS | CENTER TRIGGER

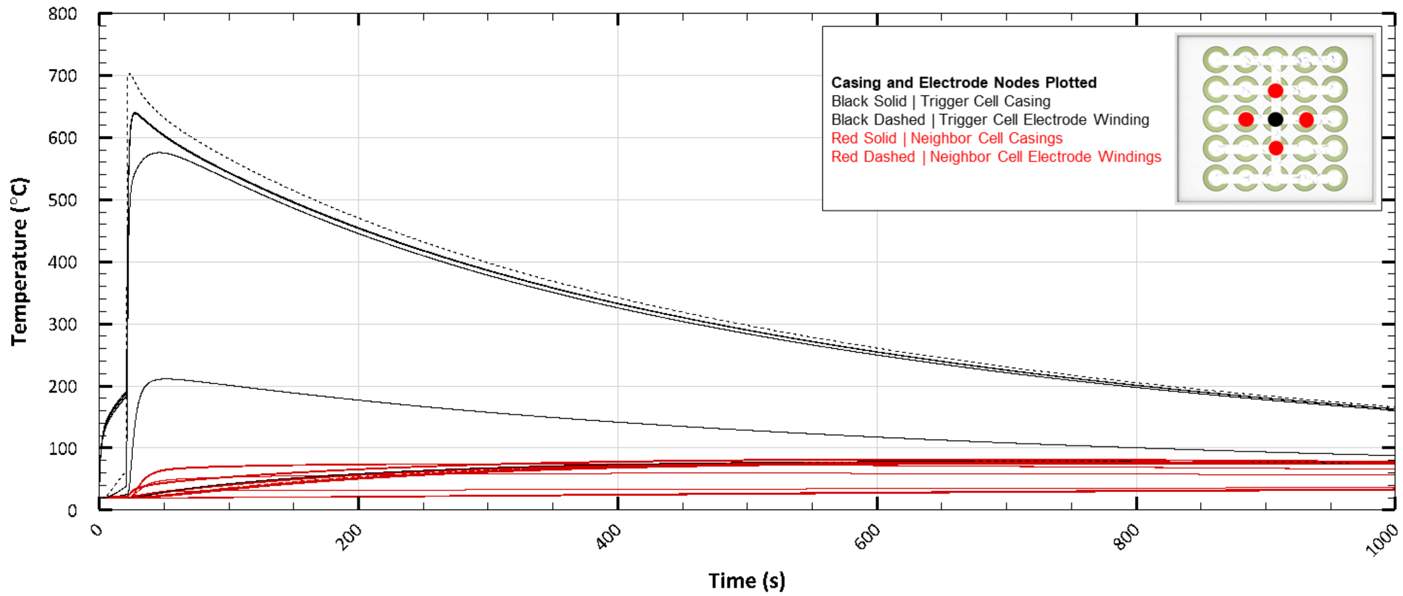
- **Results below are for the same thermal runaway conditions as previous, but for a centrally located trigger cell.**
- **Thermal simulation indicates that conditions analyzed would likely not result in cell-to-cell propagation.**
- **Why does the simulation result differ from experiment result?**
  - **Primary reason:** current lack of representation of the ejecta heat that is distributed throughout the box (temporary issue, will be added soon!).
  - **Secondary reason:** improved thermal runaway trigger criteria may be required for this non-multiphysics technique.
  - Also, important to reiterate that model correlation activities for thermal contact resistances are still ongoing.
  - Results here are still helpful for describing what a non-propagation scenario would look like and what data should be evaluated in this case.

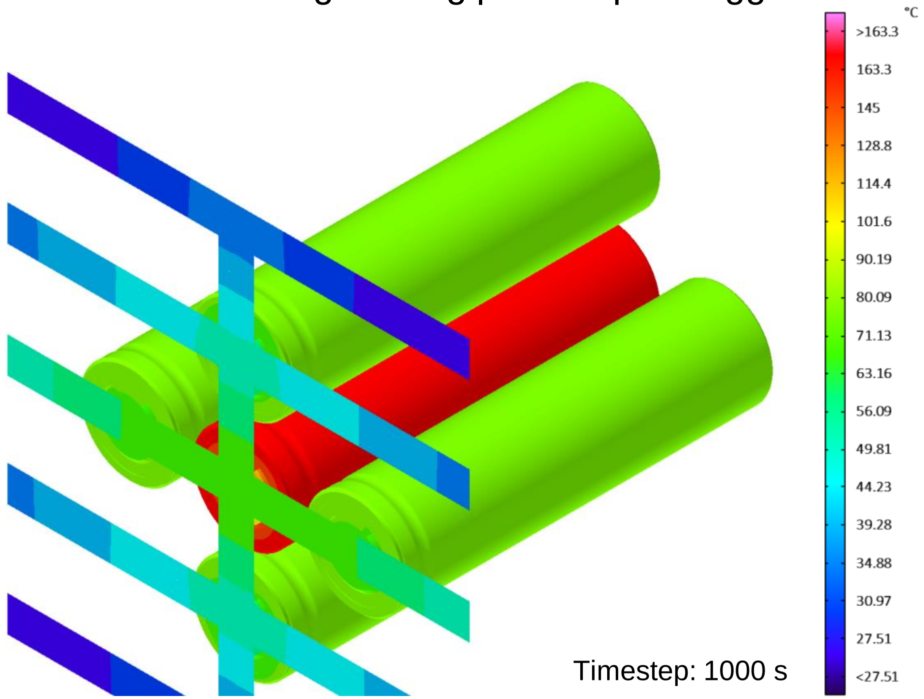




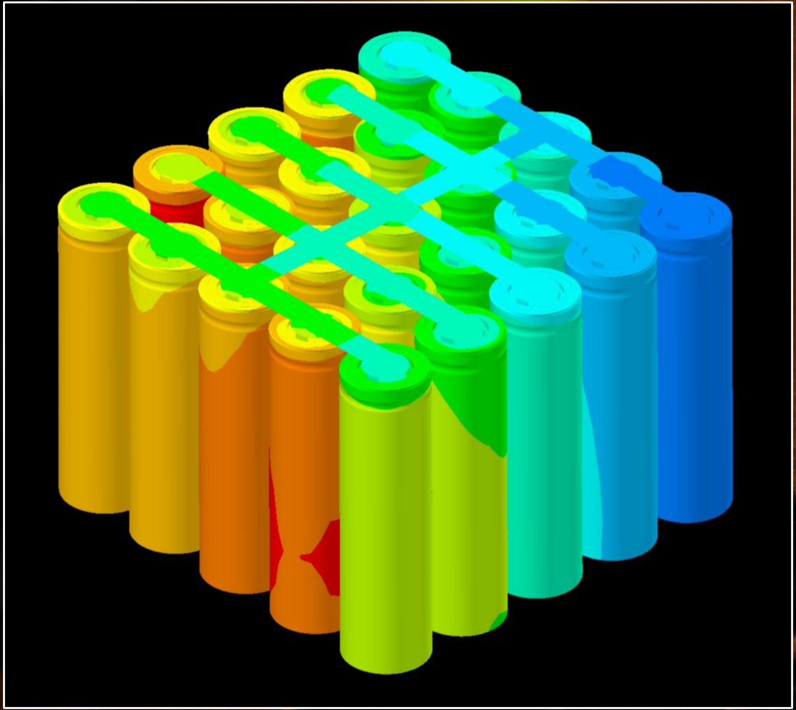
RESULTS | CENTER TRIGGER

- **As with previous case, recommend giving consideration to internal temperature profile when evaluating external temperature measurements.**
- **Central nodes from the electrode winding for the central trigger cell and neighbor cells are plotted (dashed lines) along with the corresponding cell casing lines (solid lines):**
  - Again, due to the thermal resistance between surfaces, the electrode winding is warmer than what would be ready via external temperature measurement following thermal runaway.
  - Consideration should be given to the potential gradient between cell casings and electrode windings during pre and post trigger.





Regardless of analysis technique we still have significant gaps to address between simulation and reality.



PRELIMINARY CONCLUSIONS

- **User defined distributed heat load approach offers a simplified alternative to multi-physics thermal runaway simulation that can offer useful insight into:**
  - Conductive and radiative heat transfer.
  - Design trades aimed at evaluating high conductivity vs. low conductivity thermal protection solutions.
  - Cell to cell heat transfer through interconnects and other interfacing components.
  - Likelihood of a given design to achieve propagation resistance.
- **Due to the simplified nature and reduced runtimes, parameterization is straightforward and non-computationally expensive; a combination of which can help address the variability of thermal runaway that occurs in reality that is difficult to achieve in an analysis environment.**
- **Added benefit of this technique is that it is compatible with any heat transfer analysis package that facilitates conductive heat transfer, radiative heat transfer, definition of interface thermal resistance, and user defined heat loads.**
- **Drawbacks do exist to using this approach and should not be overlooked:**
  - Inaccurate representation of the ejecta flow path and associated heating due to reliance on user defined inputs; this can make model correlation to abuse test data difficult to achieve.
  - Lack of ability to evaluate other relevant physics; e.g. flow, combustion, thermal stress, et….
  - Thermal runway is a multi-physics problem and consideration should always be given to the implications any physics being left out of the analysis.

NEXT STEPS

- **Finalize boundary conditions, geometries, and mesh combinations:**
  - Mesh should maintain strong node to node correspondence.
  - Grouping should be created to support the simulation of user defined ejecta heat loads.
- **Complete running and post-processing preliminary model checkout cases.**
- **Correlate the checked-out models to the previously conducted testing:**
  - Update thermal contact resistances based on model response.
  - Base thermal runaway heat loads on UL's previously conducted accelerating rate calorimetry (ARC) testing of the cell used for the test articles
  - Estimate energy fractions on insights provided for similar cells from the NASA and NREL hosted Battery Failure Databank.
- **Use the correlated model to help design a safe transport box that protects against thermal runaway.**
- **Evaluate the following additional areas of interest:**
  - Techniques for representing thermal runaway variability using parameterization (Monte Carlo style analysis).
  - Evaluation of time to propagation as a function of materials selection.
  - Simplified approaches to representing thermal runaway ejecta flow and combustion related heating using conduction and radiation driven software packages like Thermal Desktop®.
  - Development of recommended thermal runaway analysis guidelines – i.e. what matters most with these models and how should industry be performing these modeling activities (regardless of software package)?

Questions?

Back-Up