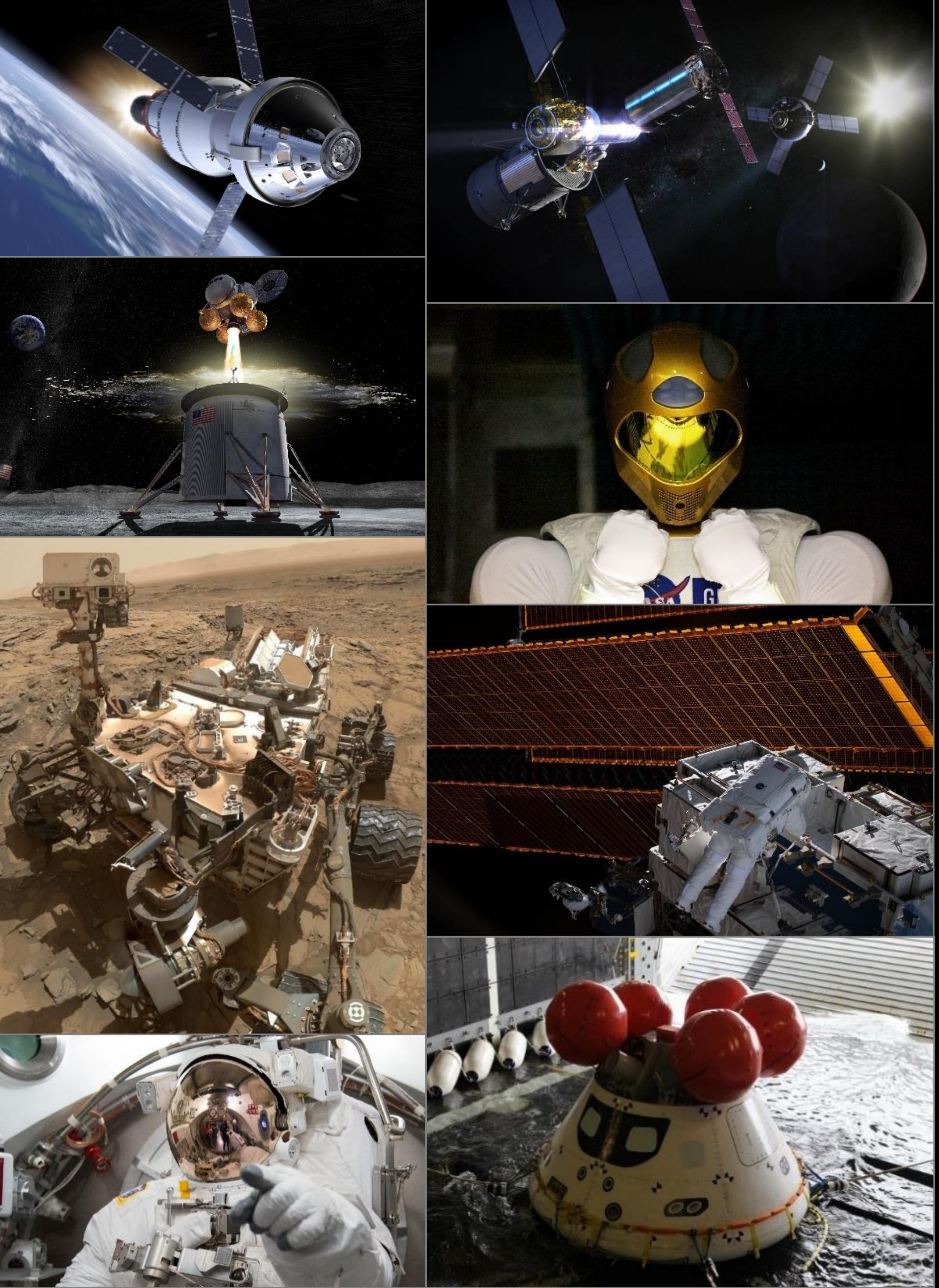

PRACTICAL BATTERY THERMAL MODELING TECHNIQUES

NASA Johnson Space Center (JSC)

Structural Engineering Division (ES) Thermal Design Branch (ES3)

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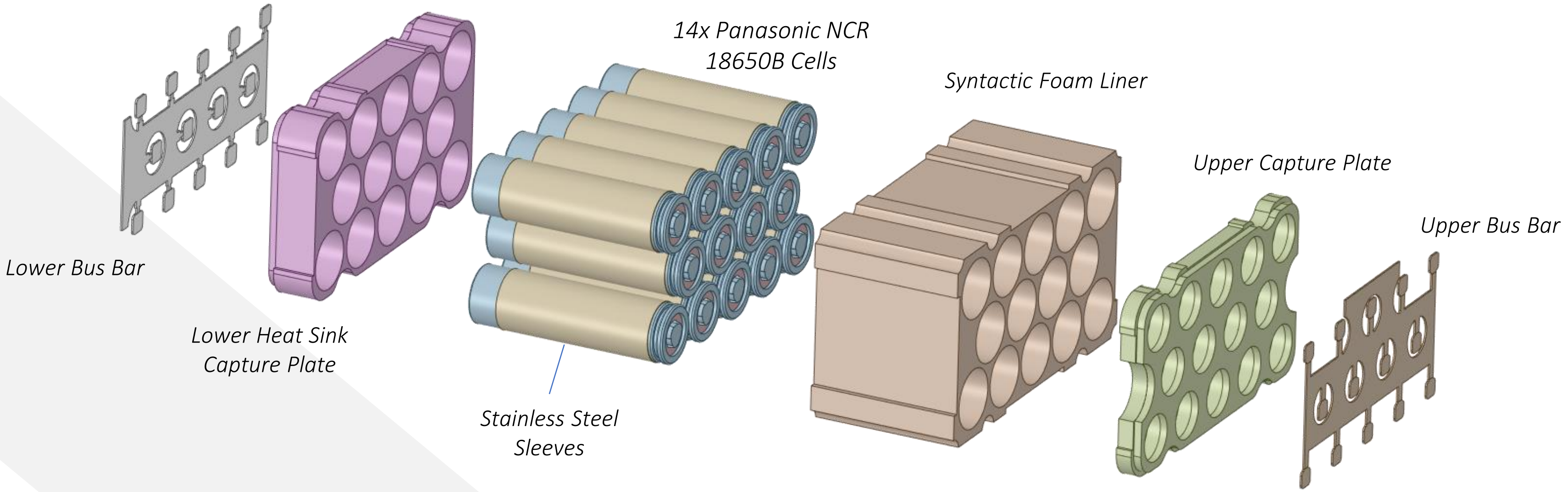
OUTLINE

- Analysis Driven Approach to Battery Design
- Battery Heat Generation
- Thermal Model Construction
- Model Development Guidelines
- Analysis
- Summary

ANALYSIS DRIVEN APPROACH TO BATTERY DESIGN

- **An analysis driven approach is often taken to develop effective Li-ion battery thermal management systems and also to characterize the general thermal performance of the overall battery assembly during design and certification phases:**
  - Various forms of thermal analysis are used to help battery designers understand system level thermal profiles as a function of battery assembly architecture in combination with cell level heating
  - This analysis can often be difficult due to the complex thermal network of a battery assembly in combination with cell level heat generation mechanisms (i.e. heat generation due to charge/discharge and heat generation due to thermal runaway)
- **This presentation was developed to provide practical battery thermal modeling techniques by using the 14-cell bank of the alternative Orion small cell battery design, as presented by Haynes et. al. (2016), as a representative geometry:**
  - A background on battery heat generation mechanisms is first provided
  - Next, a step-by-step process is presented for the construction of a thermal model of the 14-cell bank using a combination of SpaceClaim, TD Direct, and Thermal Desktop
  - Using this model, 5 Model Development Guidelines for building practical and effective battery thermal models are discussed
  - The results of a few analysis cases are also discussed, with the focus being on what results to look for and how to interpret the results
  - The intent of this presentation is to focus on “technique” rather than how to do something in a specific software package



BATTERY HEAT GENERATION: CHARGE/DISCHARGE

- **Battery design teams should understand that heat is generated when a Li-ion battery is operated; this heat generation is due to certain reversible and irreversible processes that are associated with the electrochemical reactions that drive battery charge and discharge**

- **Bernardi et. al. (1985) developed an energy balance that can be used to predict the temperature change of a Li-ion cell as a function of the following:**
  - Enthalpy of reactions and the associated entropic heating
  - Enthalpy of mixing (i.e. heat generation due to the inhomogeneous distribution of ions during charge/discharge)
  - Phase change due to diffusion of ions
  - Change in heat capacity
  - Heat associated with electrical work and over-potential
  - Heat transfer to the surroundings

- **Li-ion cell internal heat generation, due to charge/discharge, is often represented with a simplified segment of Bernardi's derivation:**

$$Q_{Cell} = I\left(V_W - V_{OC} + T\frac{dV_{OC}}{\partial T}\right)$$

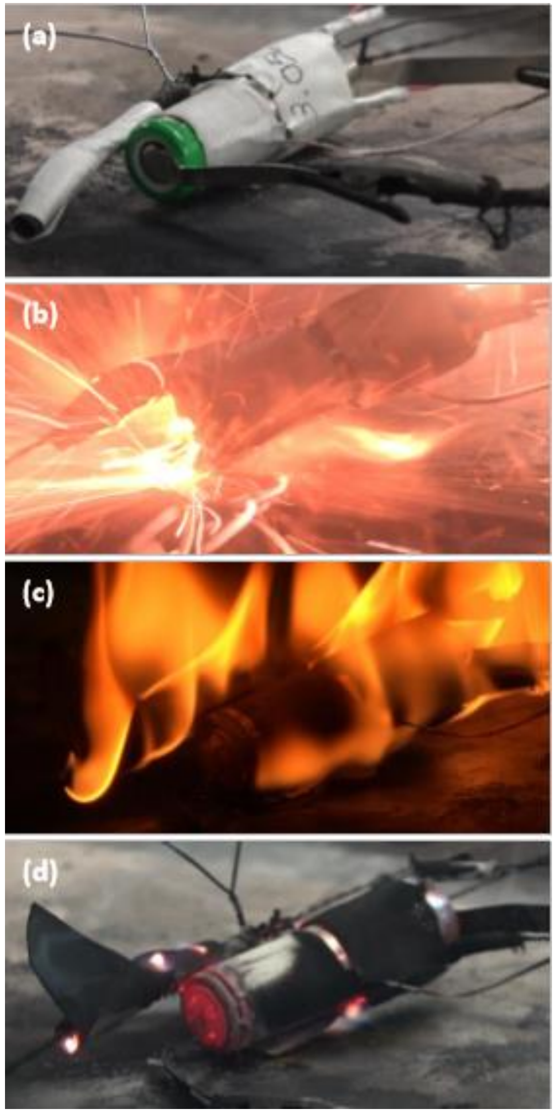
Signs based on discharge, opposite would apply for charge.

- **Unfortunately, the necessary transient voltage profiles used to solve this equation are not always available; in this case, the cell can be treated as a resistor and the heat generation can be approximated based on $\boxed{\text{Ohms law, } P = I^2R,}$ where R is the internal resistance of the cell and I is the operating current**

Information here adopted from W. Walker, "Short Course on Lithium-ion Batteries: Fundamental Concepts, Battery Safety, and Modeling Techniques," Thermal and Fluids Analysis Workshop, 2019.

BATTERY HEAT GENERATION: THERMAL RUNAWAY

- **Safety concerns exist for Li-ion battery utilization due to the possibility of thermal runaway (TR); see example to the right which depicts an 18650 cell experiencing thermal runaway (Image Credit: Walker et. al., 2019, J. Power Sources)**
- **Thermal runaway can occur when a Li-ion cell achieves elevated temperatures due to:**
  - Thermal failure (e.g. over-temp)
  - Mechanical failure (e.g. nail penetration)
  - Internal short circuiting (hard and soft variations)
  - External short circuiting
  - Electrochemical abuse (e.g. overcharge and over-discharge)
- **At elevated temperatures, exothermic decomposition reactions begin:**
  - Self-heating begins when heat generation rates exceed the heat dissipation capability
  - The rate of the exothermic reactions increase with temperature in Arrhenius form
  - Eventually, stability is lost and cell rupture and fire occurs; all remaining electrochemical energy is released
  - The models describing the decomposition reaction rates and self heating rates (i.e. kinetic relationships) are provided with the following charts
- **The severity of the event can increase if combustion between the gases released from the cell and the surrounding atmosphere is not prevented**
- **Propagation is a chain reaction event that occurs when the thermal runaway energy from an initial cell causes neighboring cells to overheat and also suffer thermal runaway failures**
- **Heat loads determined from calorimetric techniques are often used when simulating thermal runaway**



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THERMAL MODEL CONSTRUCTION: PROCESS FLOW DIAGRAM

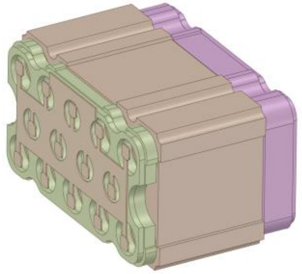
STEP 1: CREATE REFERENCE MODEL OF THE BANK COMPONENTS (REFERENCE MODEL 1)

Defeature CAD (Bus-bars, Endcaps, Interstitial Materials, Heat Sink)
SpaceClaim

Assign Domain Tag-sets for Each Set of Surface Interfaces
SpaceClaim & TD Direct

Assign Thermophysical and Optical Properties, and Radiation Analysis Groups
SpaceClaim & TD Direct

Mesh and Import into Thermal Desktop Reference Model 1
SpaceClaim, TD Direct, & Thermal Desktop

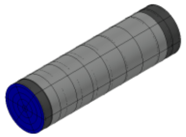


STEP 2: CREATE REFERENCE MODEL OF AN INDIVIDUAL 18650 LI-ION CELL (REFERENCE MODEL 2)

Construct Single Cell Thermal Desktop Reference Model 2 Using Native Geometries
Thermal Desktop

Assign Domain Tag-Sets for Each Set of Surface Interfaces and Each Jellyroll Solid
Thermal Desktop

Assign Thermophysical and Optical Properties, and Radiation Analysis Groups
Thermal Desktop



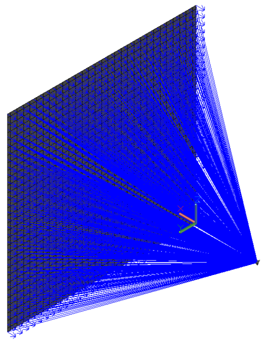
STEP 3: CREATE REFERENCE MODEL OF COLD PLATE (REFERENCE MODEL 3)

Construct cold plate in Thermal Desktop using Thermal Desktop native geometries
Thermal Desktop

Create boundary node at 25 °C
Thermal Desktop

Assign Domain Tag-sets for each interfacing surface
Thermal Desktop

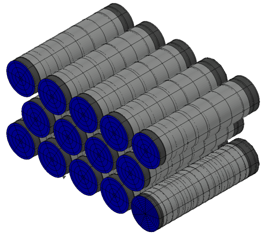
Assign thermophysical and optical properties, and radiation analysis groups
Thermal Desktop



STEP 4: CREATE REFERENCE MODEL OF GEOMETRIES REPRESENTING CELL PLACEMENT LOCATIONS (REFERENCE MODEL 4)

Use defeatured CAD to create geometry representing cell locations
SpaceClaim

Import Geometries into Thermal Desktop Reference Model 4
Thermal Desktop

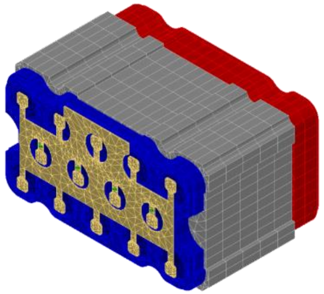


STEP 5: CREATE MASTER MODEL THAT COMBINES ALL REFERENCE MODELS VIA XREF

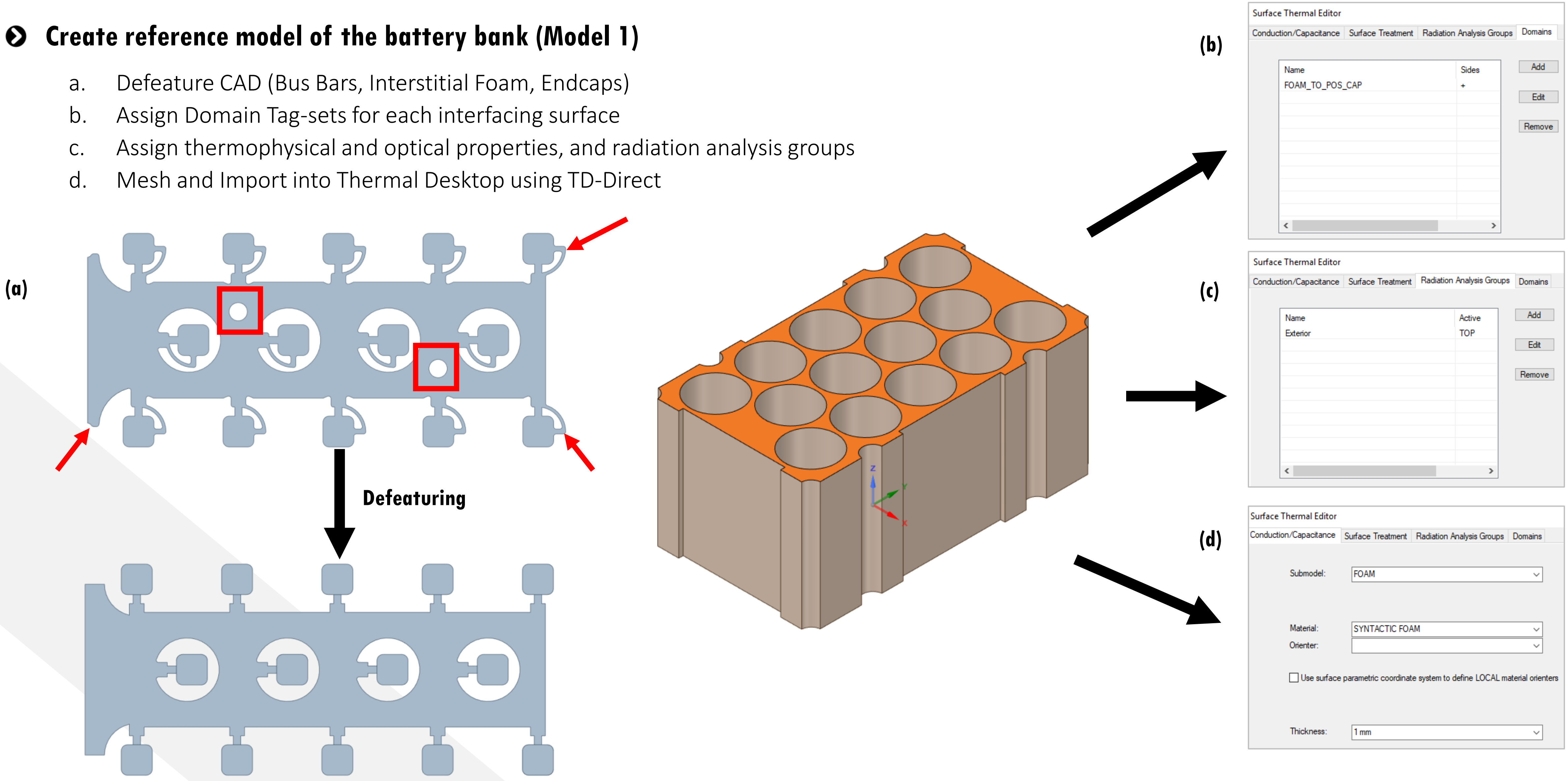
Use TD-Direct to import the battery bank (Model 1) and the cell placement geometry (Model 4)
Thermal Desktop

Use XREF to place an individual 18650 cell (Model 2) at each cell location on the placement geometry (Model 4)
Thermal Desktop

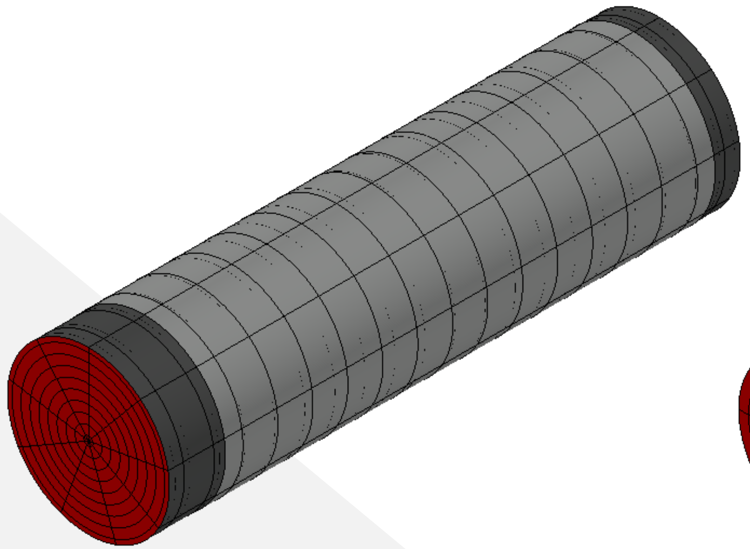
Use XREF to import cold plate (Model 3)
Thermal Desktop



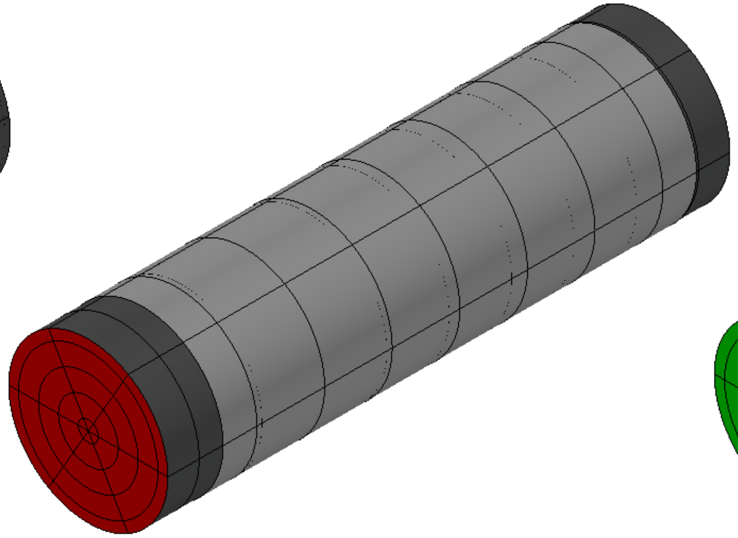
- **Create reference model of the battery bank (Model 1)**
  a. Defeature CAD (Bus Bars, Interstitial Foam, Endcaps)
  b. Assign Domain Tag-sets for each interfacing surface
  c. Assign thermophysical and optical properties, and radiation analysis groups
  d. Mesh and Import into Thermal Desktop using TD-Direct



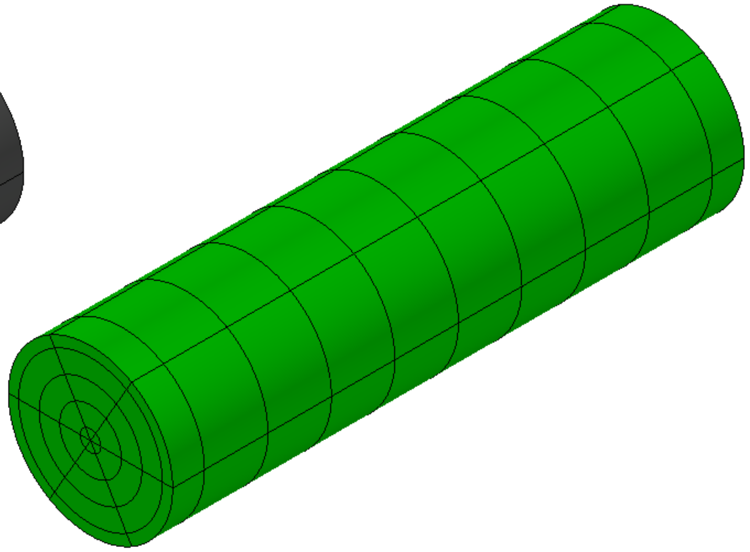
- **Create reference model of an 18650 Li-ion cell (Model 2)**
  - Build single cell Thermal Desktop reference model using Thermal Desktop native geometries, including distinct jellyroll geometry
  - Assign Domain Tag-sets for each interfacing surface
  - Assign thermophysical and optical properties, and radiation analysis groups



18650 Trigger Cell Casing/Sleeve



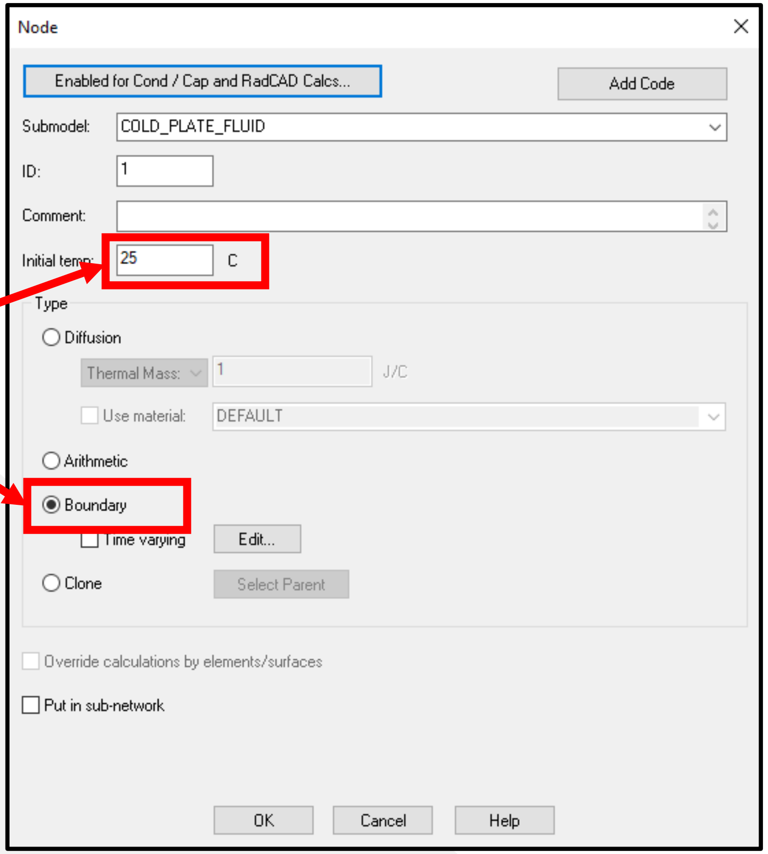
18650 Reference Cell Casing/Sleeve

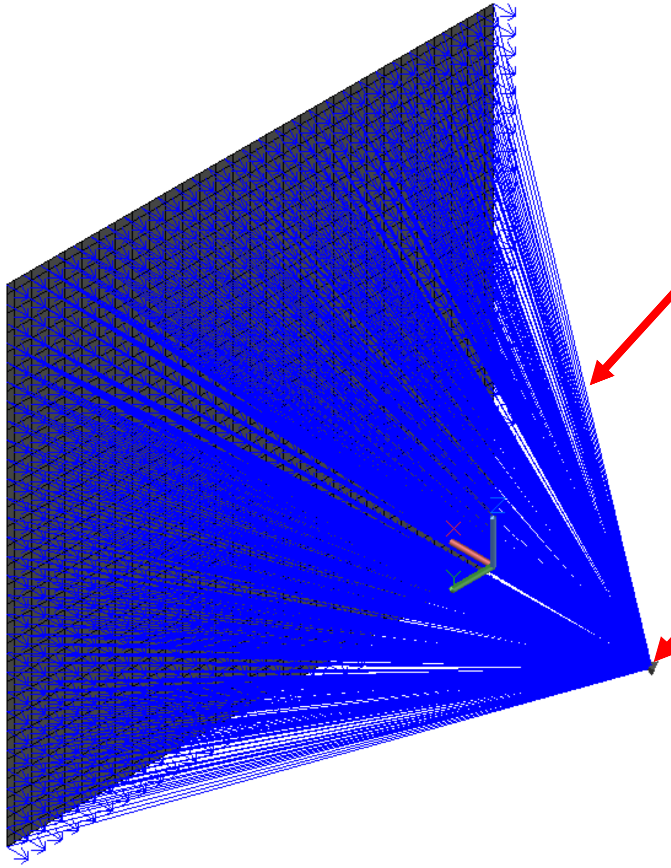


18650 Jellyroll

- **Create reference model of cold plate (Model 3)**
  - Construct cold plate in Thermal Desktop using Thermal Desktop native geometries
  - Create boundary node at 25 °C
  - Assign Domain Tag-sets for each interfacing surface
  - Assign thermophysical and optical properties, and radiation analysis groups

Convection to 25 °C



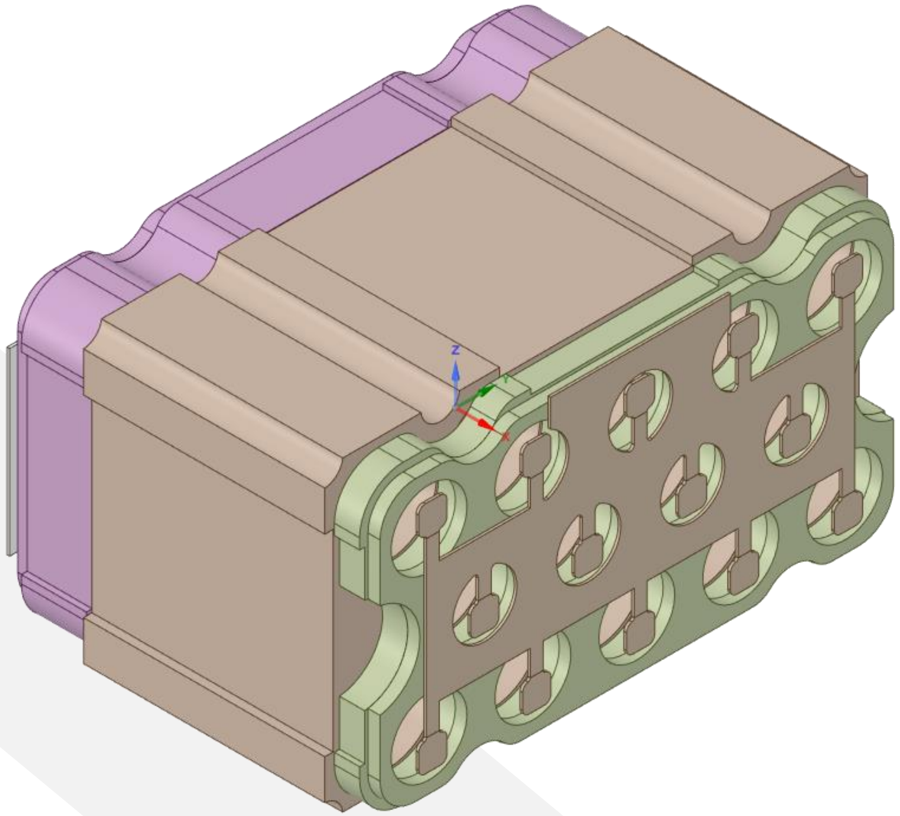


Convection from cold plate

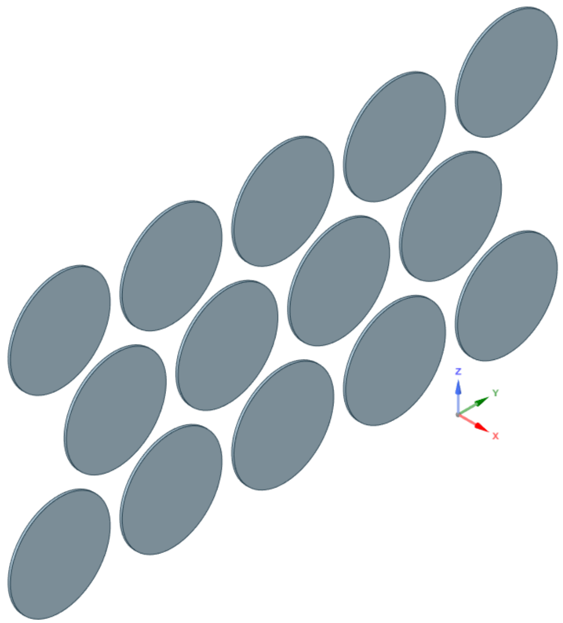
Boundary Node

THERMAL MODEL CONSTRUCTION: STEP 4

- **Create reference model for cell placement on the cell (Model 4)**
  - Use defeatured CAD to create geometry representing cell locations (used to locate 18650 cells in Thermal Desktop XREF feature)
  - Import into Thermal Desktop using TD-Direct



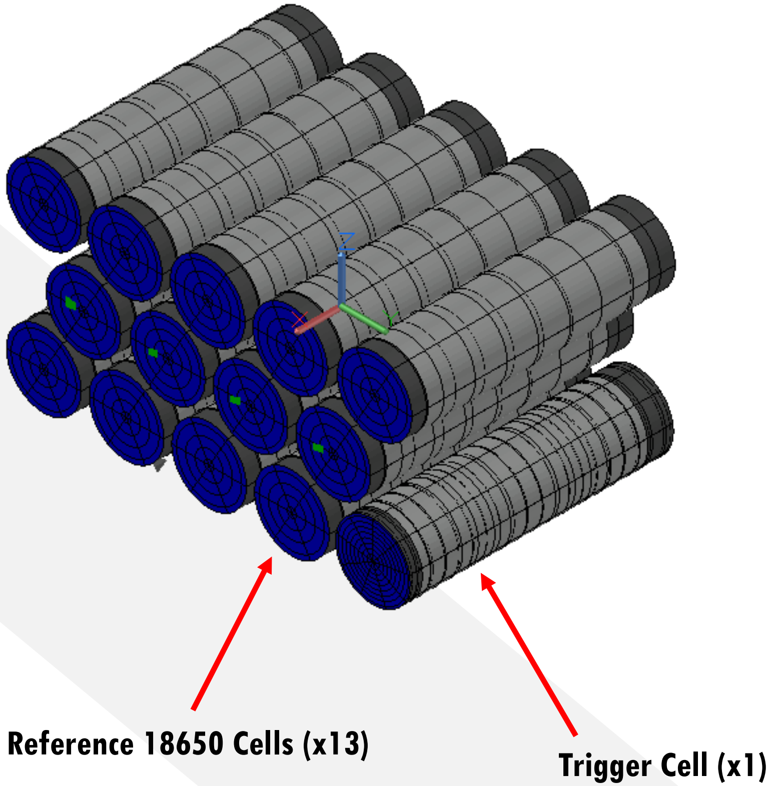
Original 14-cell CAD

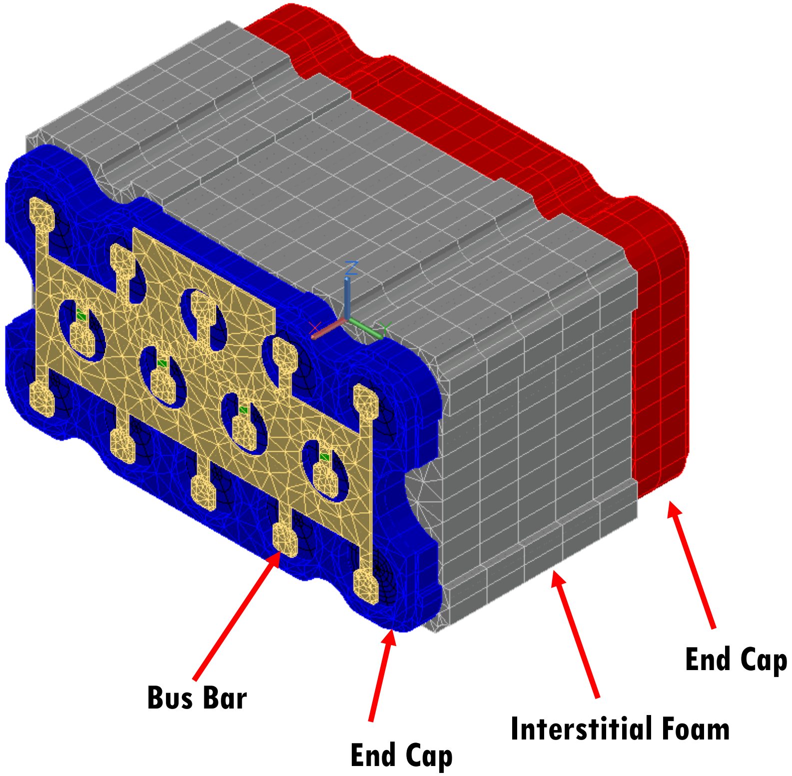


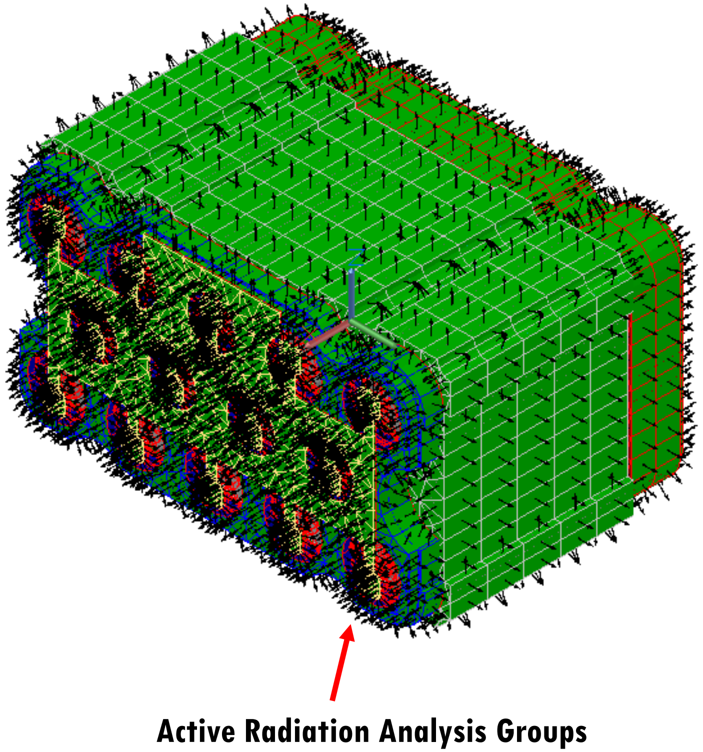
Cell Placement Geometry derived from 14 cell design

THERMAL MODEL CONSTRUCTION: STEP 5

- **Create a master model in Thermal Desktop using TD Direct and XREF**
  - Use TD-Direct to import the battery bank (Model 1) and the cell placement geometry (Model 4)
  - Use XREF to place an individual 18650 cell (Model 2) at each cell location on the placement geometry (Model 4)
  - Use XREF to import cold plate (Model 3)







MODEL DEVELOPMENT GUIDELINES

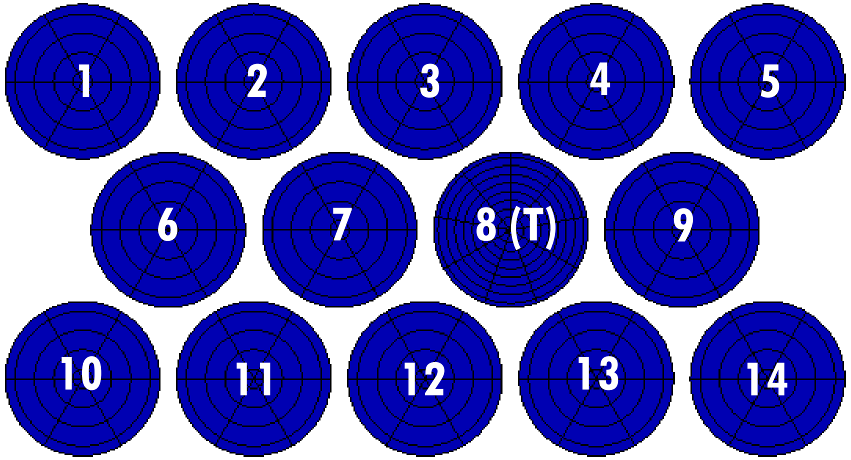
1. **Organization is Key:**
   - Use an organized and easily understood naming/numbering convention for banks and cells

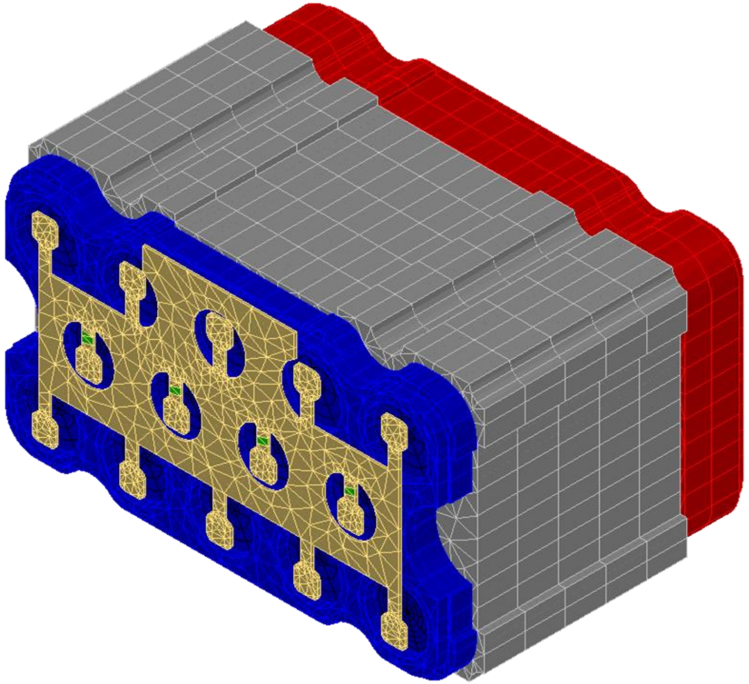
2. **Model Distinct Battery Features:**
   - Ensure that cell models have distinct jellyrolls and cell casings
   - Gaitonde et. al. (2017) provides reference for the interface resistance value

3. **Create a Flexible Model:**
   - Model architecture to support frequent changes to re-use geometries
   - Ex: 18650 cells are reused through the XREF feature

4. **Utilize Grouping Utilities:**
   - Establish easily-accessible groups of surfaces and elements for contacting geometries
   - Ex: Specify domain tags in SpaceClaim or Thermal Desktop before importing model

5. **Differentiate Bulk and Cell-Specific Jellyrolls:**
   - Have direct access and controls over bulk jellyroll heat loads and specific jellyroll heat loads
   - Ex: Bulk control over jellyroll heat loads used for charge/discharge profile, whereas cell-specific control used for thermal runaway trigger cells





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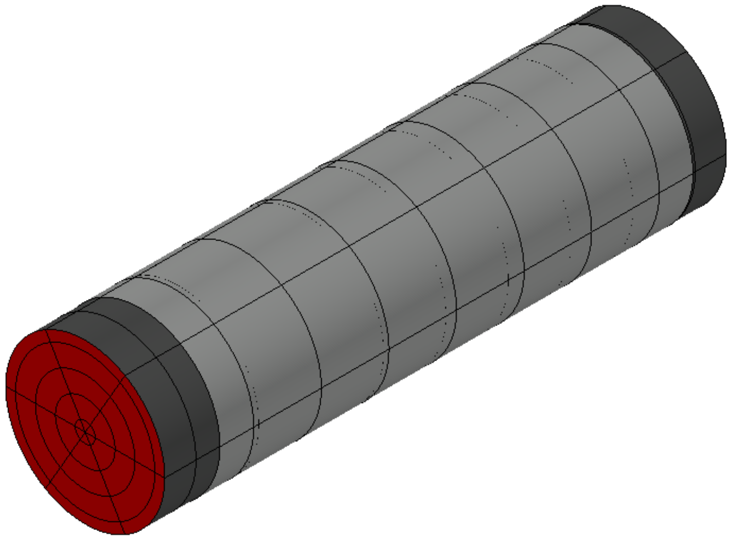
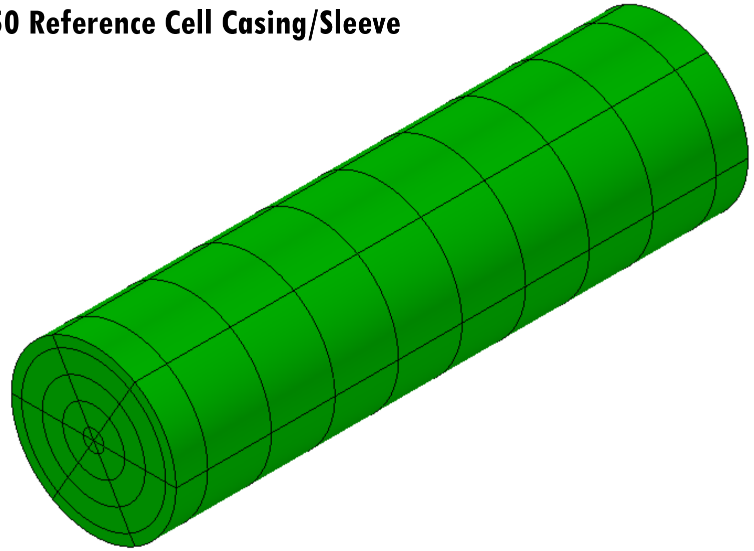


18650 Reference Cell Casing/Sleeve



18650 Reference Jellyroll

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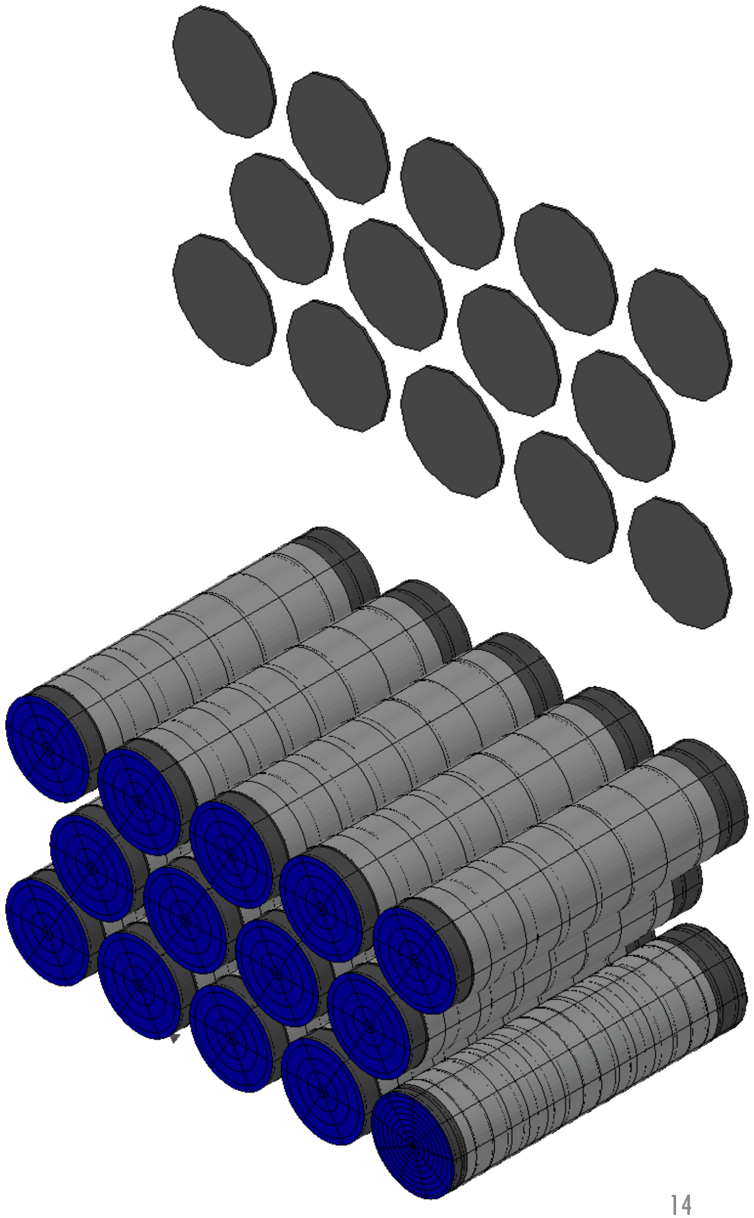

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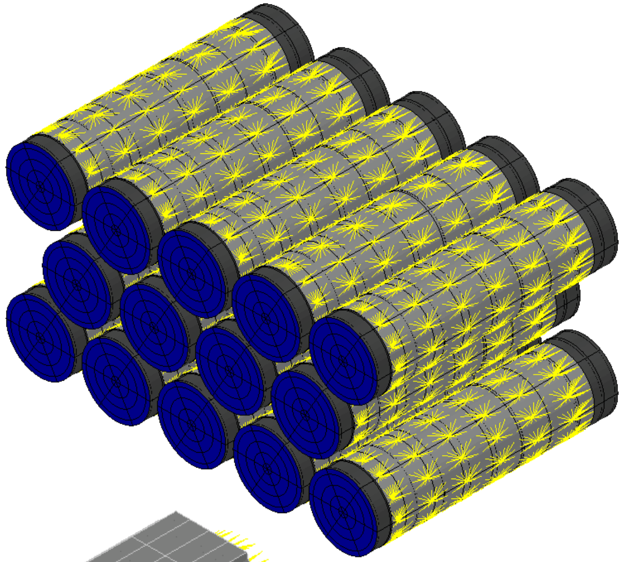

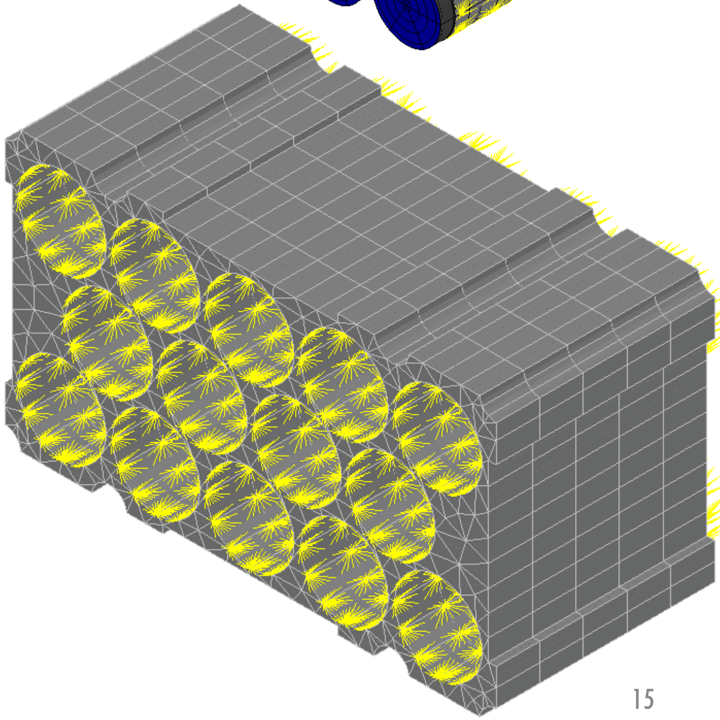

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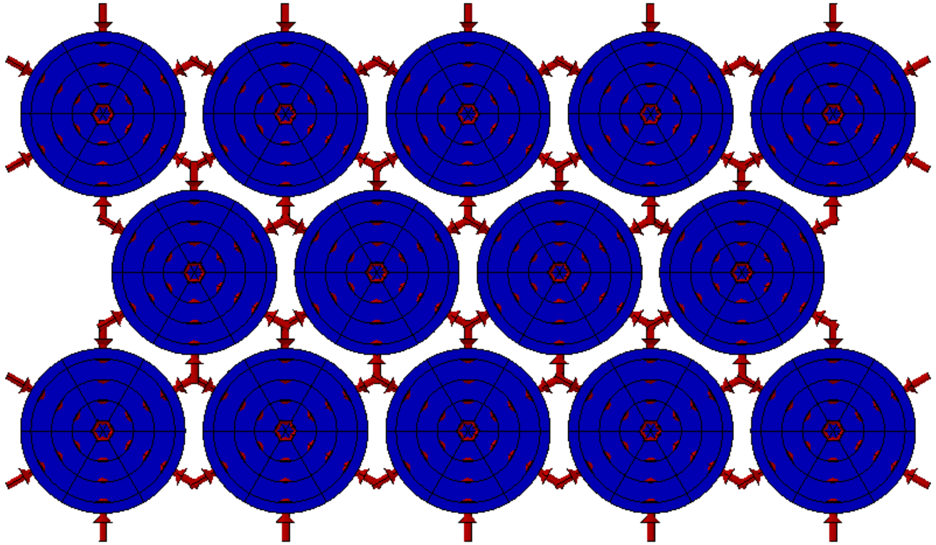
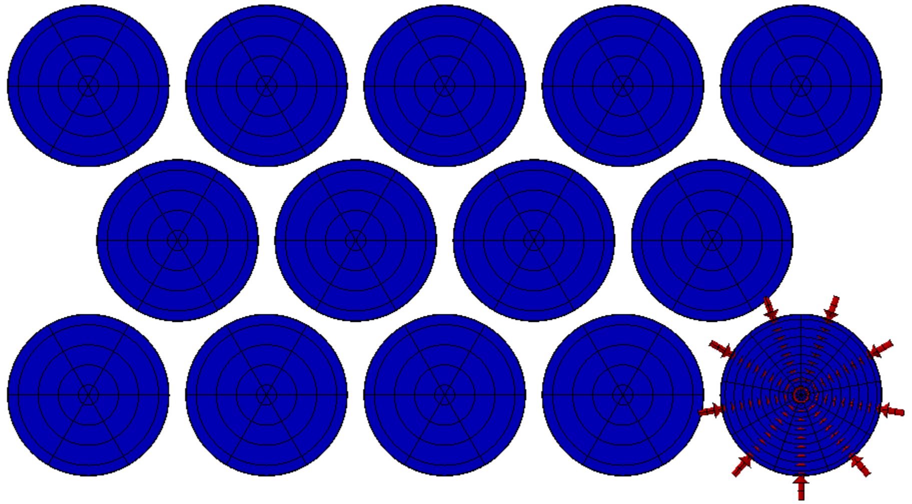
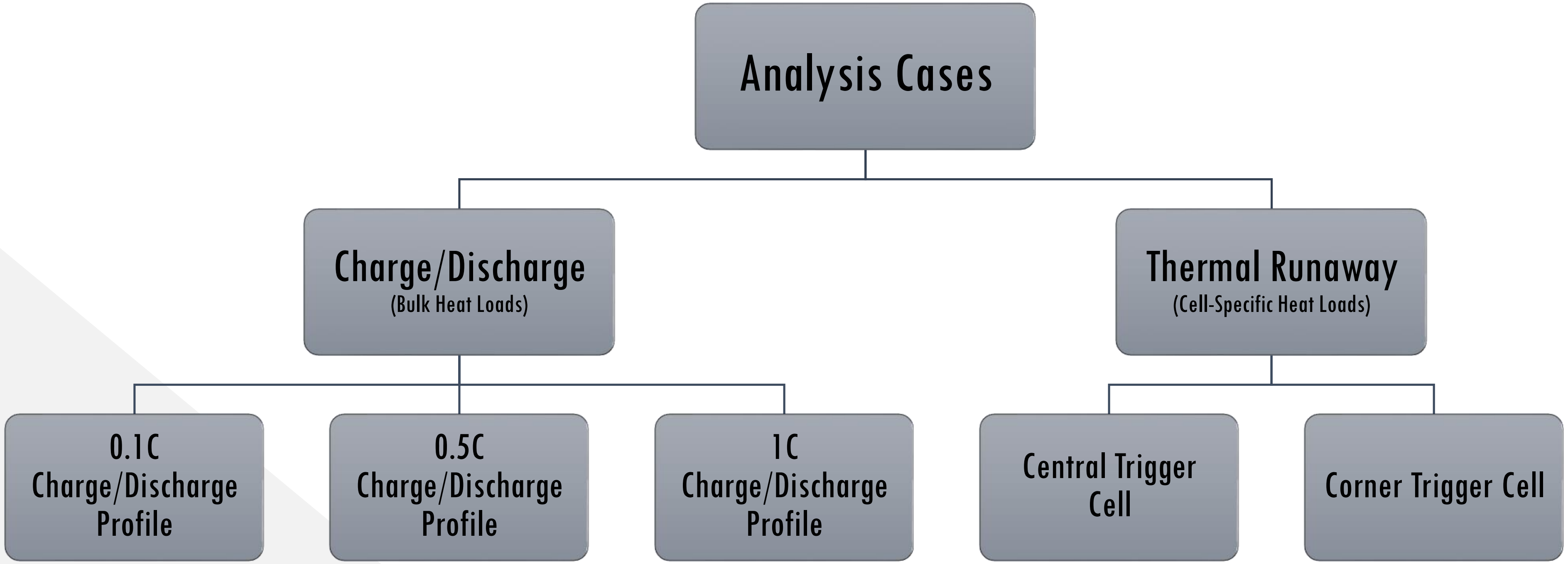




ANALYSIS- EXAMPLE CASES

- **Boundary Conditions:**
  - Nodes initialized at 25°C
  - Cold plate underneath heat sink maintained at 25°C
  - Radiative sink temperature of 25 °C
- **Analysis Cases:**
  - Representative of charge/discharge heat loads, and thermal runaway events



ANALYSIS- CHARGE/DISCHARGE PROFILES

- **Heat Profile determined via $P = I^2R$ relationship to represent charge or discharge**
  - Should be treated as an approximation for quick turnaround analysis; more extensive analysis should consider the effects of overpotential and entropic heating (Bernardi, et. al. 1985)
  - Cell internal resistance estimated from Chen & Shen (2017)
- **Important for bank to operate at close to uniform temperature to prevent undesired degradation**
- **Analysis allows for studying the jellyroll vs. cell casing temperatures**

C-Rate	Current (A)	Internal Resistance (Ω)	Heat Load per Cell (W)	Total Bank Heat Load (W)
0.1C	0.335	0.075	0.118	1.65
0.5C	1.675	0.075	2.946	41.24
1.0C	3.350	0.075	11.784	164.97

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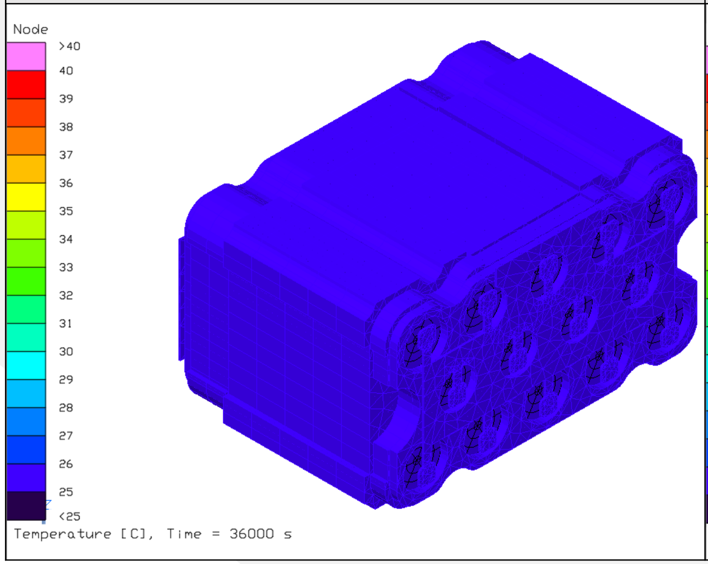
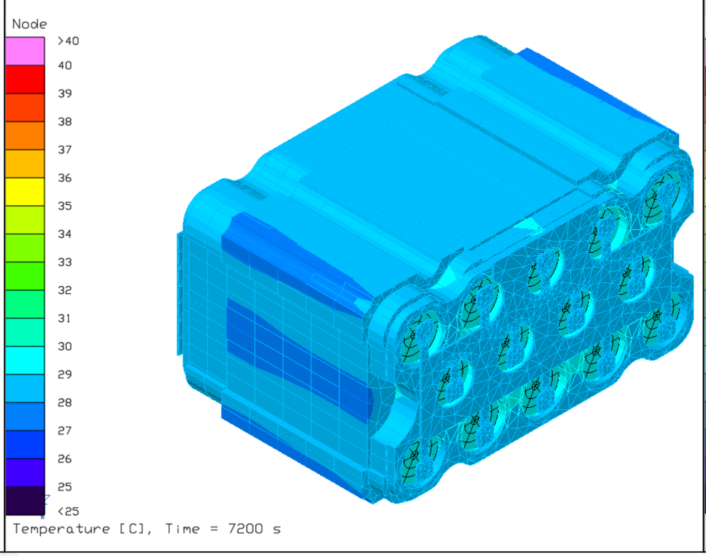
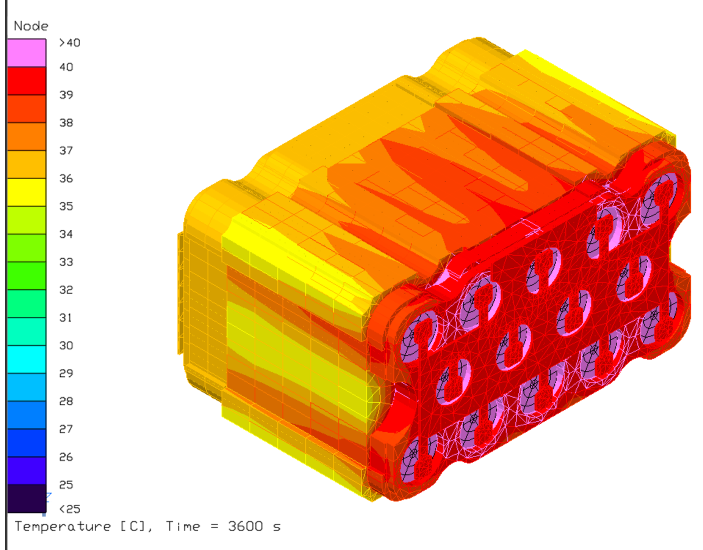
0.1C Charge/Discharge Profile	0.5C Charge/Discharge Profile	1.0C Charge/Discharge Profile







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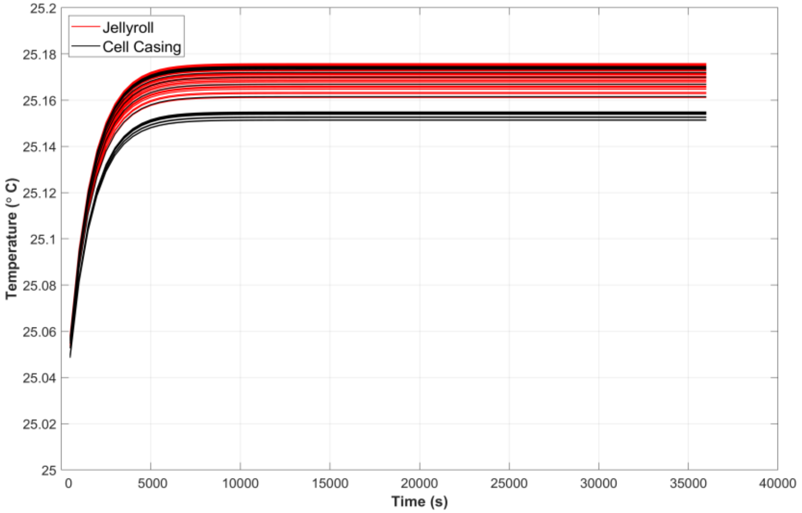
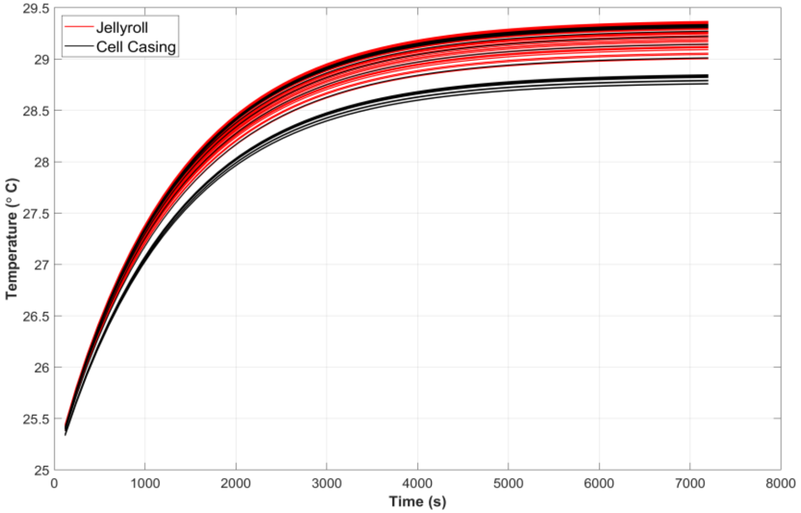
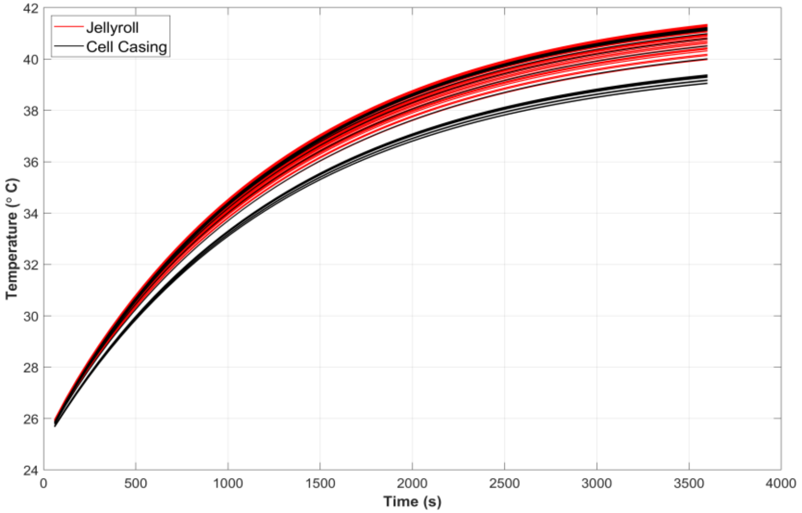
0.1C Charge/Discharge Profile

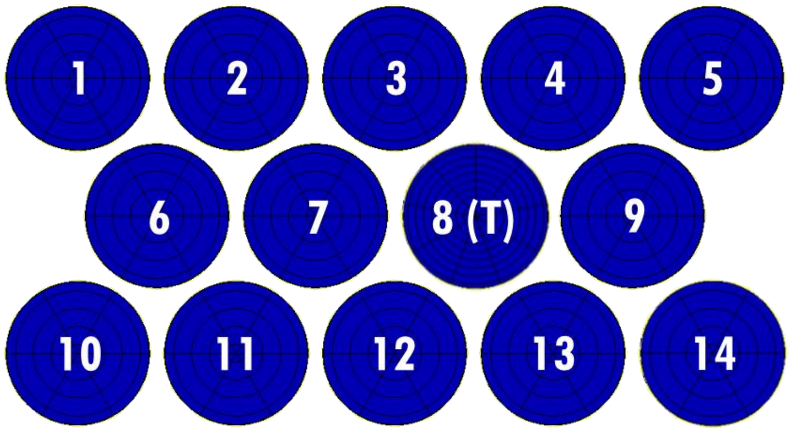


0.5C Charge/Discharge Profile

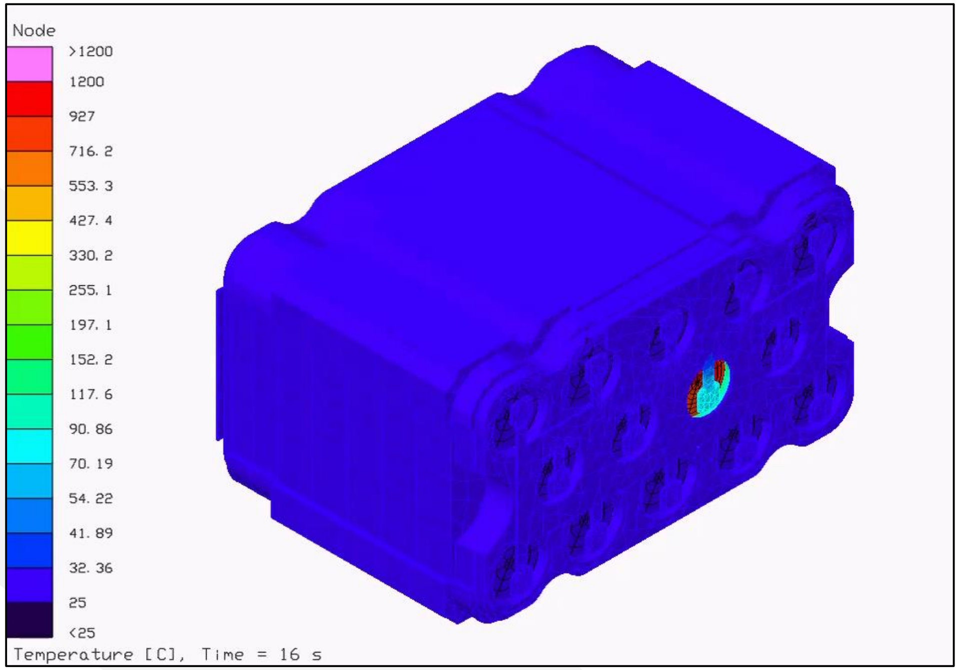


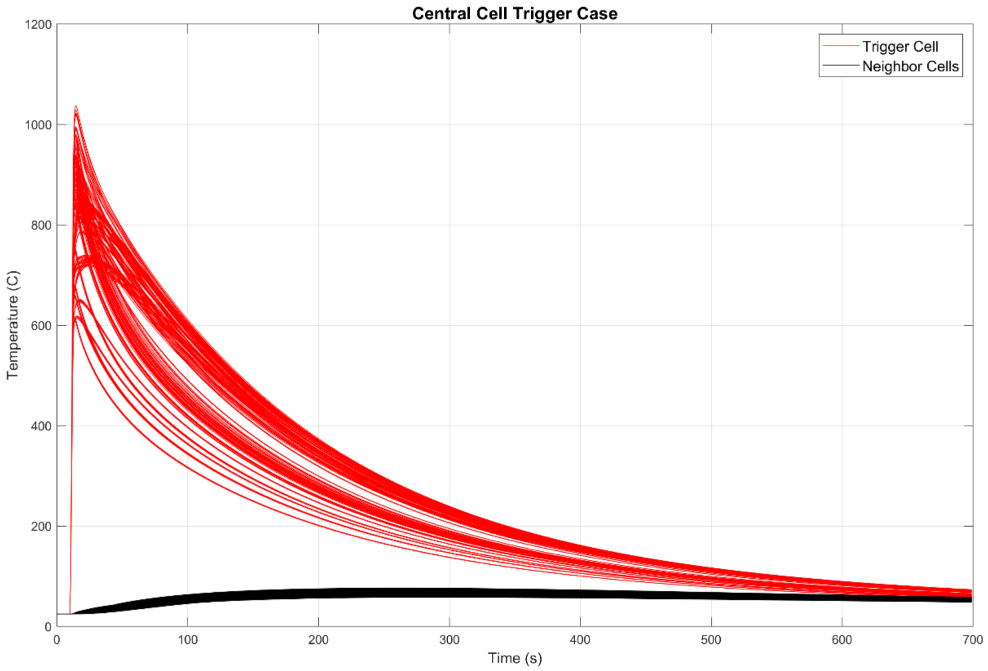
1.0C Charge/Discharge Profile





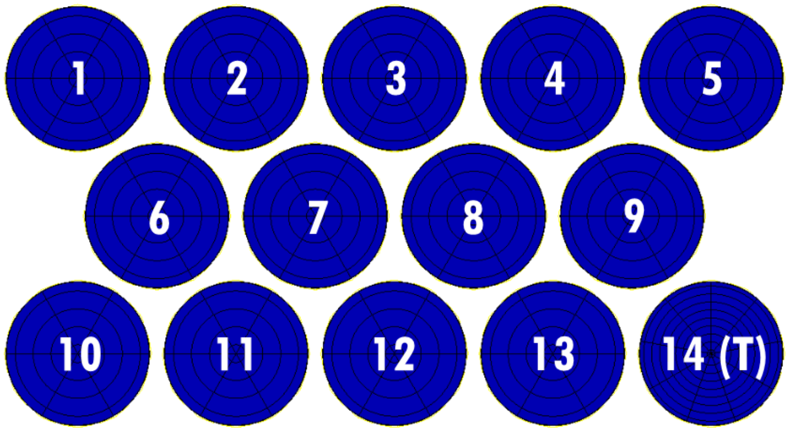
- **Heat load**
    - 50 kJ applied to trigger cell jellyroll over two second period
- **Things to consider when post-processing:**
    - Movement of heat throughout the battery pack as a whole
    - Trigger cell temperature (both cell casing and jellyroll)
    - Neighbor cell temperatures (both cell casing and jellyroll)
    - Variability in all of the above as a function of thermal runaway heat distribution
    - Ability to post-process nodes that correspond to installed thermocouple locations when comparing to test data

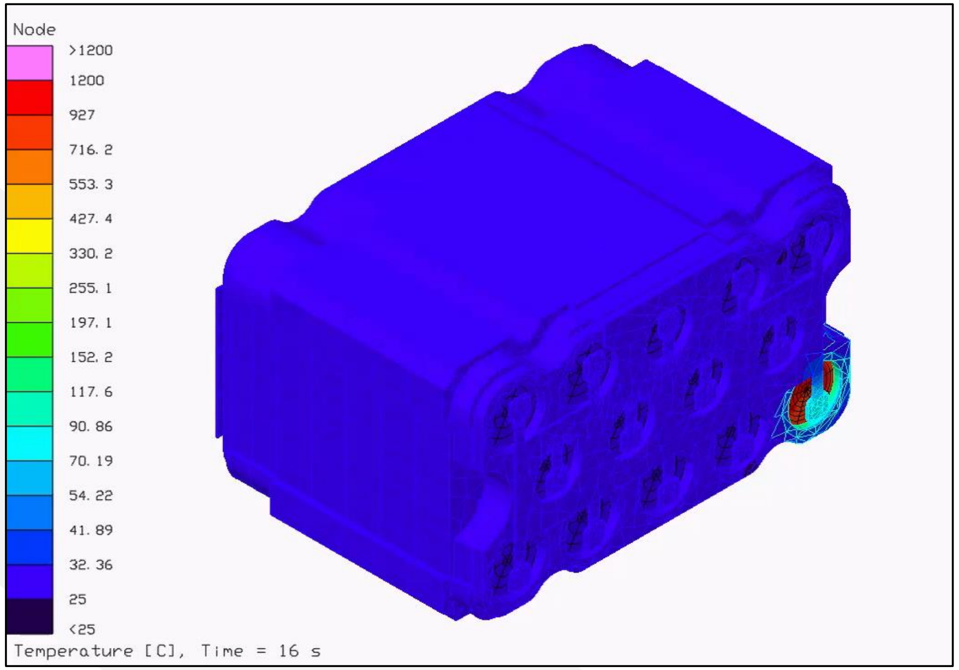


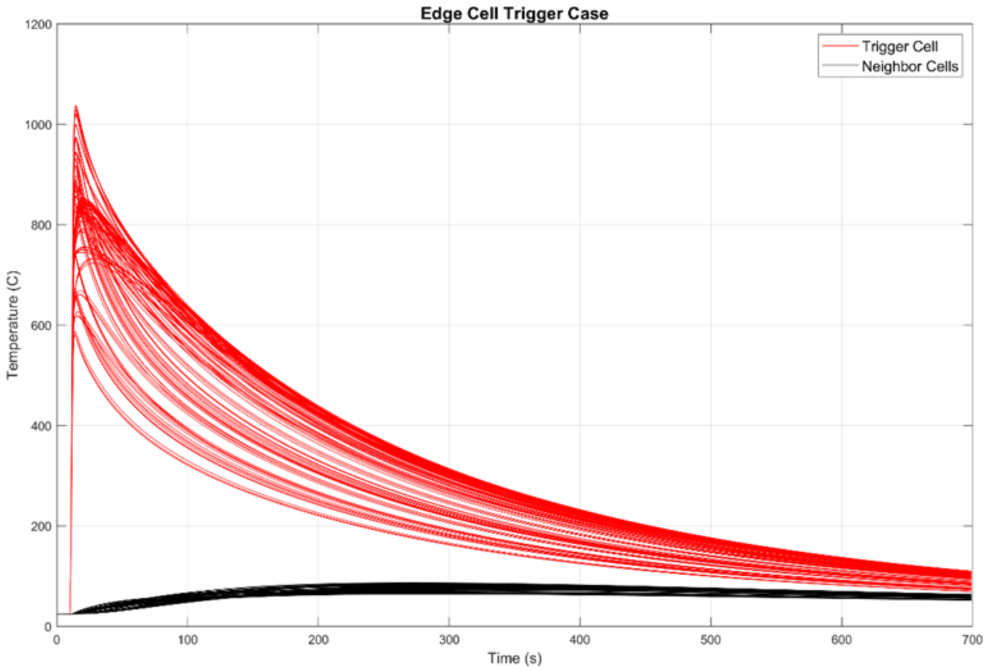


ANALYSIS- THERMAL RUNAWAY, EDGE CELL TRIGGER

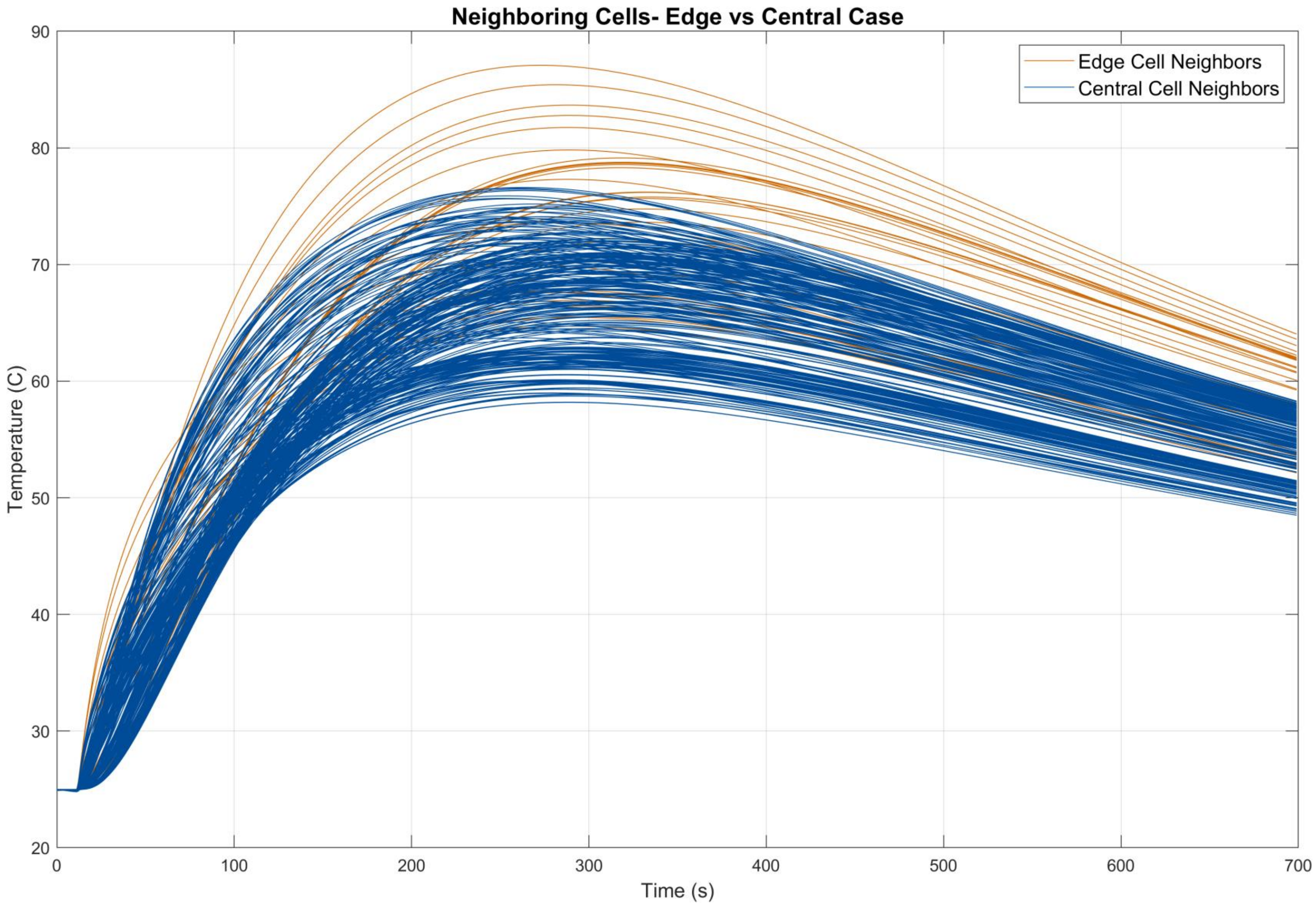
- **Heat load**
  - 50 kJ applied to trigger cell jellyroll over two second period
- **Things to consider when post-processing:**
  - Movement of heat throughout the battery pack as a whole
  - Trigger cell temperature (both cell casing and jellyroll)
  - Neighbor cell temperatures (both cell casing and jellyroll)
  - Variability in all of the above as a function of thermal runaway heat distribution
  - Ability to post-process nodes that correspond to installed thermocouple locations when comparing to test data



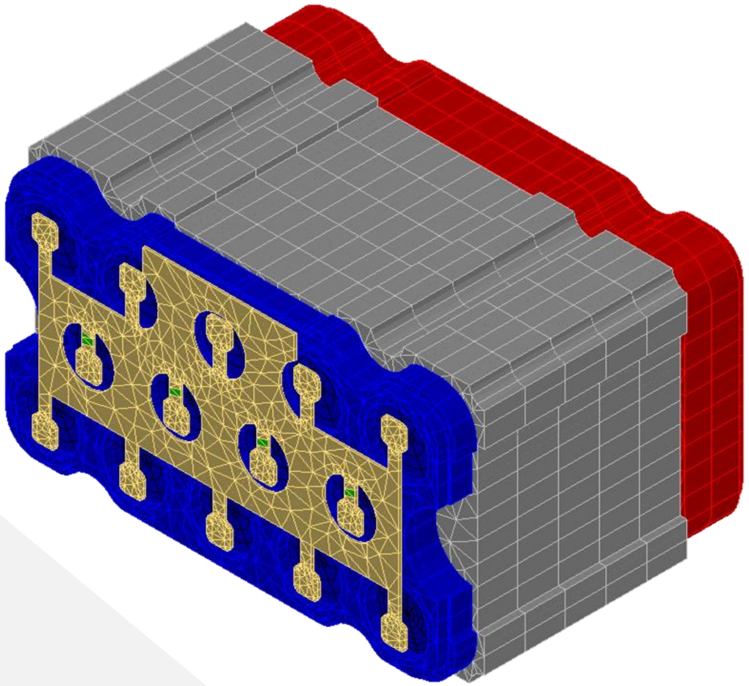




- **When analyzing a thermal runaway event, a variety of cases should be considered, ranging from edge cell thermal runaway to central cell thermal runaway.**
  - From a cell-to-cell propagation standpoint, edge cell thermal runaway tends to be the worst case scenario.
  - In this example, neighbor cells for the edge case get 10°C hotter than those for the central trigger cell case (under the same thermal runaway conditions). This can mean the difference between passing or failing an abuse test, depending on the pass/fail criteria.
- **Test-correlated analysis can be used to help battery designers understand the difference between test data gathered with temperature sensors and the overall system-level response**



SUMMARY



Model Construction	Create reference model of the battery bank
	Create reference model of an 18650 Li-ion cell
	Create reference model of cold plate
	Create reference model for cell placement on the cell
	Create a master model in Thermal Desktop using TD Direct and XREF
Practical & Effective Modeling Guidelines	1) Organization is key
	2) Model distinct battery features
	3) Create a flexible model
	4) Utilize grouping utilities
	5) Differentiate bulk and cell-specific jellyrolls
Charge/ Discharge Analysis	Charge/Discharge Profiles can be determined via $P = I^2R$ relationship or Bernardi method
	Analysis allows for investigation of bank gradients at different heat loads
	Jellyroll and cell casing temperatures should be compared
Thermal Runaway Analysis	Edge trigger cell and central trigger cell cases should be considered
	From a cell-to-cell propagation standpoint, edge cell thermal runaway tends to be the worst case scenario
	Temperature profiles of cells neighboring the trigger cell should be investigated

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