Modeling Li-Ion Batteries with CRTech’s Thermal Desktop®

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Battery Thermal Analysis Techniques
Short-course Addendum
Abstract

While modeling the electrochemical phenomena in lithium-ion batteries is important at some level, approximations of the exothermic and endothermic heating in the cells allow evaluating the thermal behavior in a cell-, subsystem-, or system-level model using CRTech's Thermal Desktop. We will present the modeling procedure for creating a 14-cell block of 18650-format Li-ion cells along with a separation material and capture plates above and below the cells using the Thermal Desktop suite of tools. The results presented will show the thermal behavior of the system while charging and discharging and the thermal behavior during thermal runaway events in an exterior and an interior cell. Features of the tool suite that benefit the analysis of battery packs will be highlighted.
Overall Procedure

1. Create a model of single cell
   - This model will be referenced as a TD Block Reference that can be updated in one location

2. Create a model of the block configuration
   1. Create (or import and simplify) the geometry in SpaceClaim
   2. Mark up the geometry with modeling information (material names, submodels, surface properties and domains)
   3. Mark up the geometry with mesh controls
   4. Import to Thermal Desktop

3. Reference the single cell model and copy 14 times
4. Add additional geometry (sleeves), boundary conditions, heat loads, contactors, and user logic for the heat load calculations
5. Define the case set by setting symbols to activate and deactivate various model behaviors
   - For example, setting RunawayCell to a positive value identifies the cell that will experience thermal runaway
Charging to Full Charge
Discharging to Minimum Charge
Runaway on Edge Cell

Runaway Cell 1

Temperature, °C

Time, s

Temperature (°C), Time = 100 s
Runaway on Center Cell
Features of Interest

Quick updates

- Parameterization
  - Geometry dimensions can be parameterized to easily make updates
  - Other values, such as contact conductances, can be parameterized for uncertainties
    - Automatic test data correlations can minimize the error between model results and test data by changing identified uncertainties – match phenomena not included in the solution
    - Model-to-model correlations can improve reduced-resolution models for system-level studies
- Material aliases
  - Objects can be assigned material alias names to easily change the assigned materials when a design is not mature or trade studies must be performed
- TD Direct mesh updates
  - Thermal connections made through domains (TD Direct markups) are reapplied if the mesh is updated due to resolution changes or geometry modifications
Features of Interest

- **Quick updates**
  - TD Block References
    - Multiple instances of an item can be controlled by a single file
    - When the referenced file is updated, all copies of that reference are updated
    - Can be reused in various configurations
Features of Interest

- **User customization**
  - The solution can be customized to meet the analysis needs
    - Thermal Desktop does not include electrochemical phenomena, but assumptions can be added to the solution through user customization
    - In addition to writing logic and adding subroutines, User-Defined Fortran Arrays allow creating your own variables for nodes, conductors, or any network object.

- **Initializing results**
  - One solution can be initialized from another solution so solutions can be combined
    - A thermal runaway solution can be initialized from the point on orbit where the temperature is maximum without rerunning the orbit scenario
OpenTD API

- OpenTD API can quickly generate multiple versions of the same component
  - The following demonstration shows the cells (jellyrolls, canisters, and heat-load terms) being added to the block after specifying the dimensions and counts in the pattern
  - Programs can be reused to create a library of complex components
    - When building a model once, TD Block References work well
    - If the configuration changes often, programming the cell creation can pay off.

Note: The following program was created by a relatively inexperienced OpenTD programmer in about 5 hours
OpenTD demo: Populating cells

Each cell is in its own submodel
So we don’t neglect FloCAD®

A flow battery


A single cell in a 17-cell stack in a 6-stack battery over the course of a day
References

- FOAMGLAS® ONE™ data sheet, Pittsburgh Corning