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Designing Safe Lithium-Ion Battery Packs Using Thermal Abuse Models

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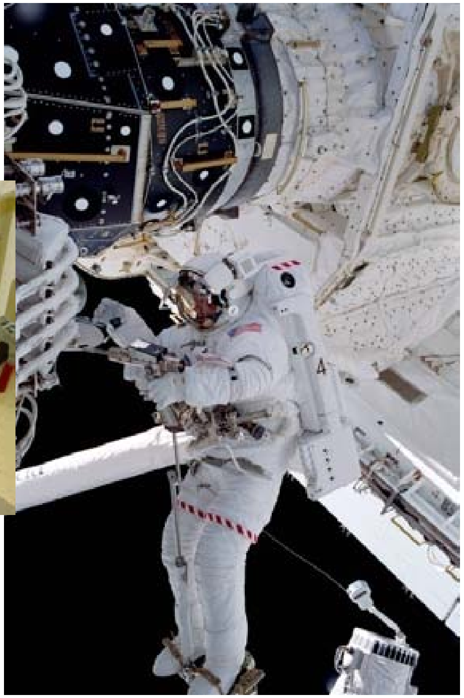
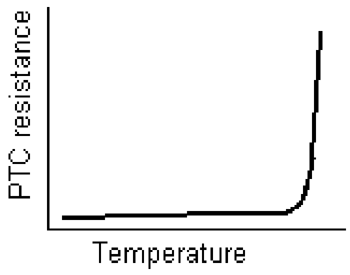
Background

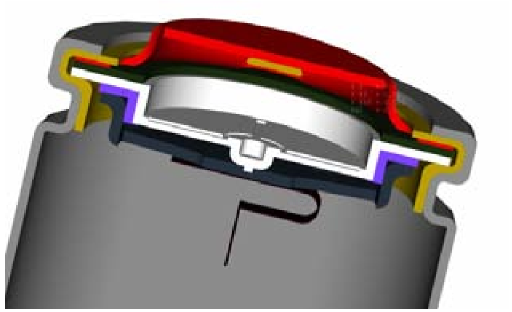
- For powering spacesuits, NASA is considering using a battery pack consisting of arrays (16P-5S) of 18650 Li-ion cells.
- These cells are equipped with a positive temperature coefficient (PTC) device proven effective for control of overcurrent hazards at the Li-ion cell and small battery level.
- However, PTC devices are not as effective in high-voltage battery designs.
- A fire in a 2004 Memphis FedEx facility suspected to be due to a PTC device failure in a large-capacity (66p-2s) battery shorted while at 50% SOC.



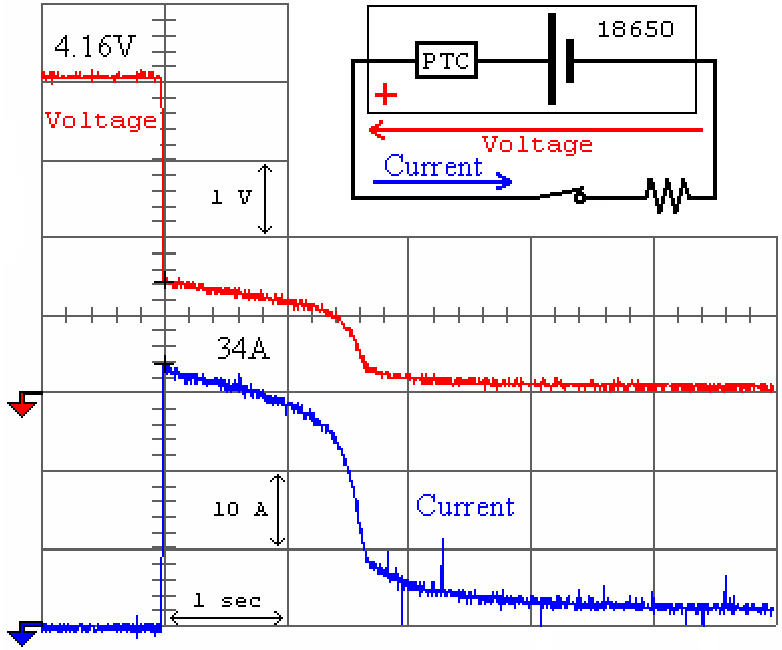
PTC Device: Background

- Commercial lithium-ion 18650 cells typically have a current-limiting PTC (positive temperature coefficient) device installed in the cell cap to limit external currents in the event of an external short to the cell.
- The PTC device consists of a matrix of a crystalline polyethylene containing dispersed conductive particles, usually carbon black.* The resistance of the PTC device increases with temperature.
- The PTC resistance increases sharply with temperature. When a short is applied to a cell, the elevated currents cause the PTC to self-heat and move to a high-resistance state in which most of the cell voltage is across the PTC but the current is significantly reduced.
- As long as the short is maintained, the PTC device produces enough heat to keep itself in this tripped state (lower current is offset by greater voltage drop across PTC).



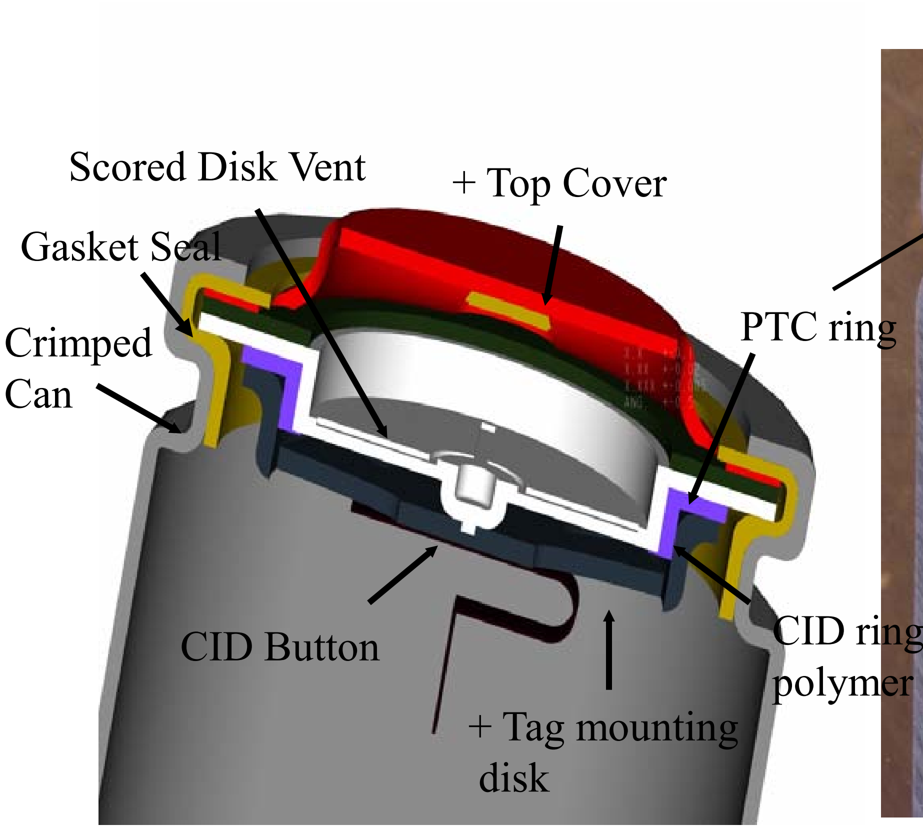


Single Cell Short:

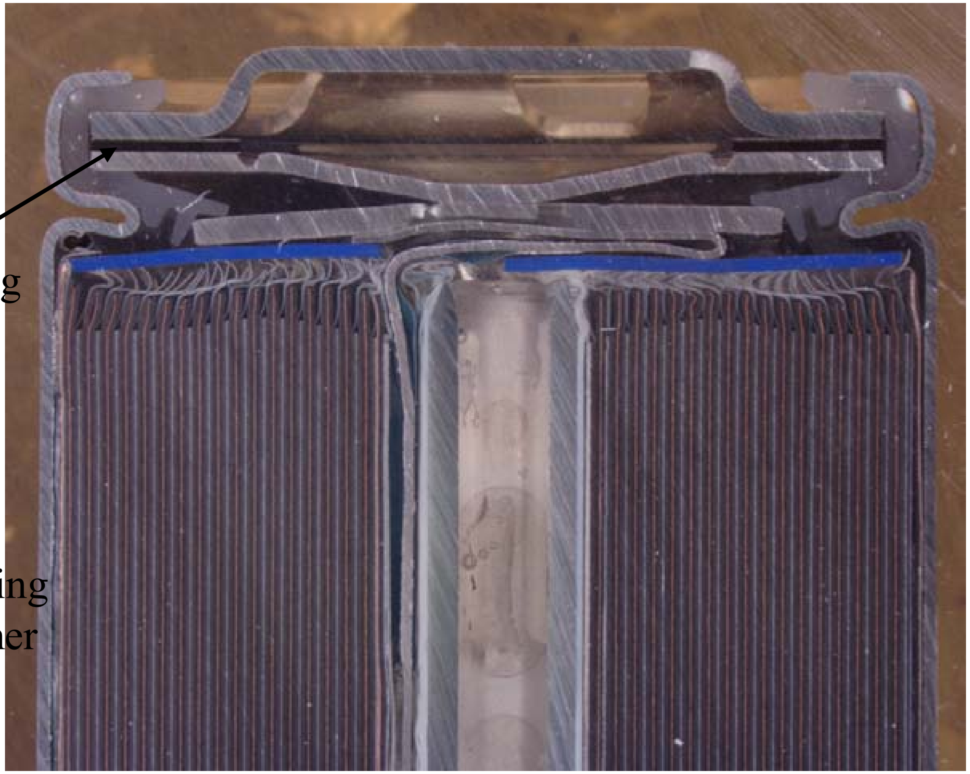


*Doljack, F., IEEE Transactions on Components, Hybrids, and Manufacturing Technology, **4**, 732, 1981

Cell Design Features for Abuse Tolerance



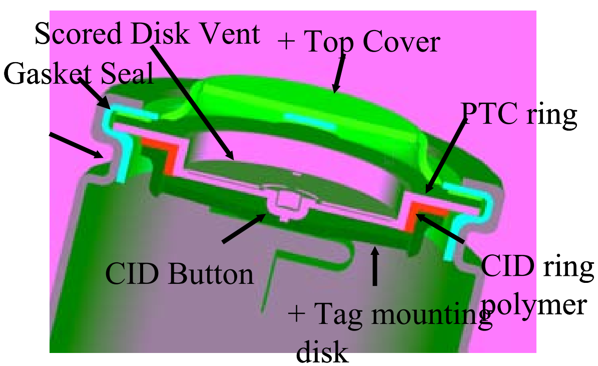
Sony HC Cell

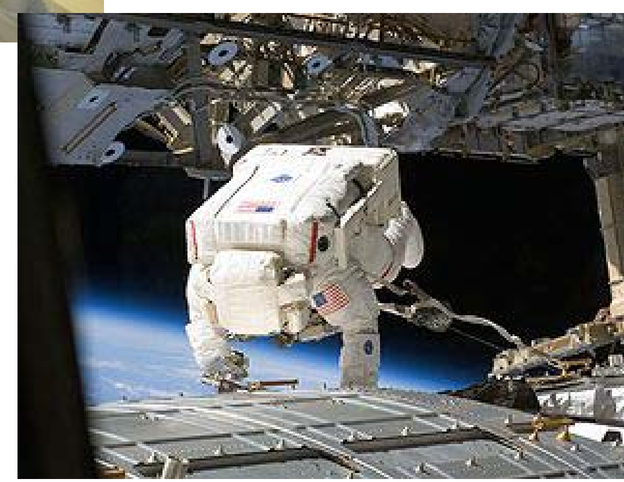


Moli ICR-18650J

Motivation for this Work

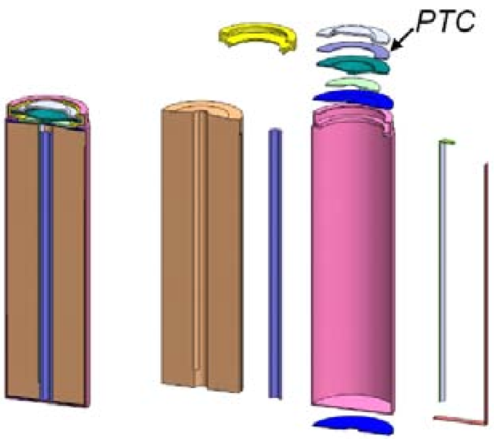
- Can NASA's spacesuit battery design (16p-5s) array depend on cell PTC devices to tolerate an external 16p short?
- Is there a range of smart shorts that can be hazardous?





Objectives

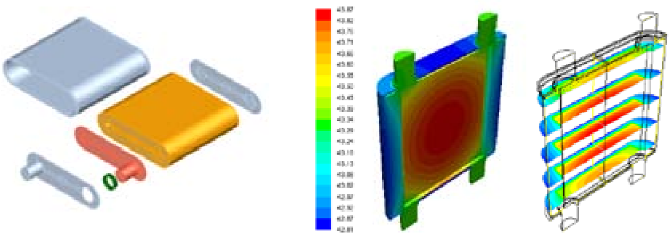
- Create an engineering model to guide the design and to verify the safety margin of a battery using high specific energy COTS cells

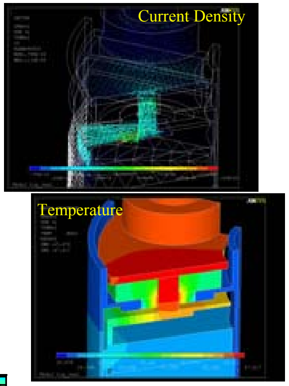


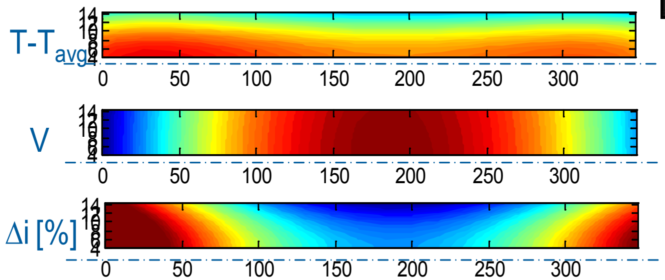
- Use the model to provide input for designing a NASA 16p-5s 18650 spacesuit battery
  - Cell model must include the electrical and thermal behavior of the cell PTC device
  - Use cell model as building block to model multi-cell battery behavior under short-circuit conditions
  - Assess the range of smart short conditions that push cells close to the onset of thermal runaway temperature

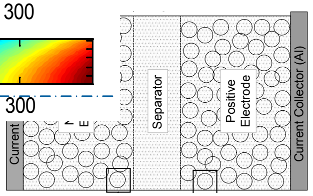
Utilizing NREL’s Multi-physics Battery Modeling

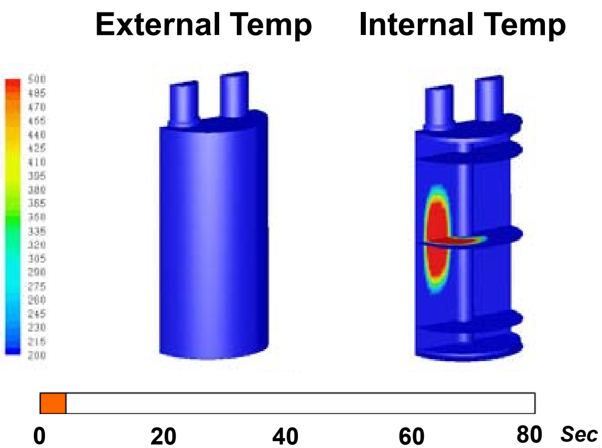
- Electrical Performance Modeling
  - Cells & multi-string modules
- Thermal Modeling
  - Cells & modules
- Thermal/Electrochemical Modeling
  - Cells
- Thermal/Chemical Abuse Modeling*
  - Cells and modules

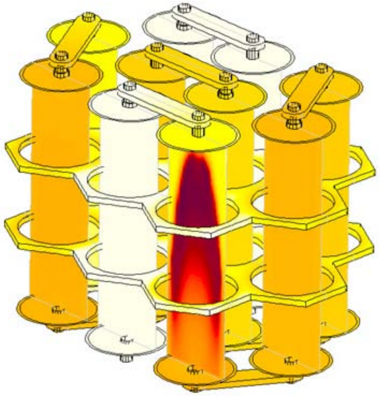


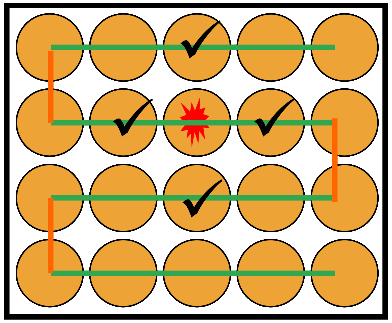








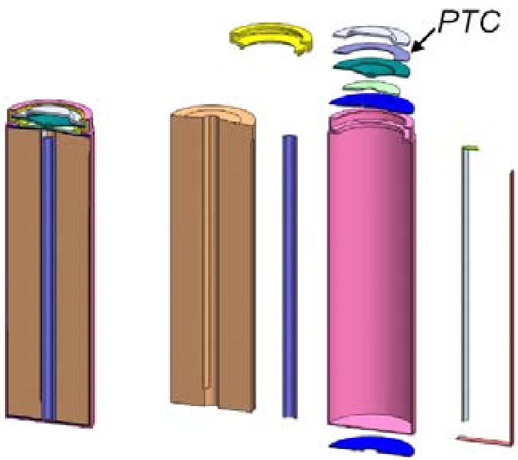




*G.-H. Kim, A. Pesaran, “Analysis of heat dissipation in Li-ion cells and modules for modeling of thermal runaway,” 3rd International Symposium on Large Lithium Ion Battery Technology and Application, Long Beach, CA, May 2007. Available: www.nrel.gov/vehiclesandfuels/energystorage/

Overview

- Modeling
  - Approach
  - PTC device
  - Cell
    - Electrical
    - Thermal (5-node)
  - Module
    - Electrical (multi-node network)
    - Thermal (multi-node network)
- Validation with experiments from SRI
  - 16P module with 10 mΩ external short
- Parametric study
  - Resistance of external short
  - Heat rejection rate to ambient
- Conclusions



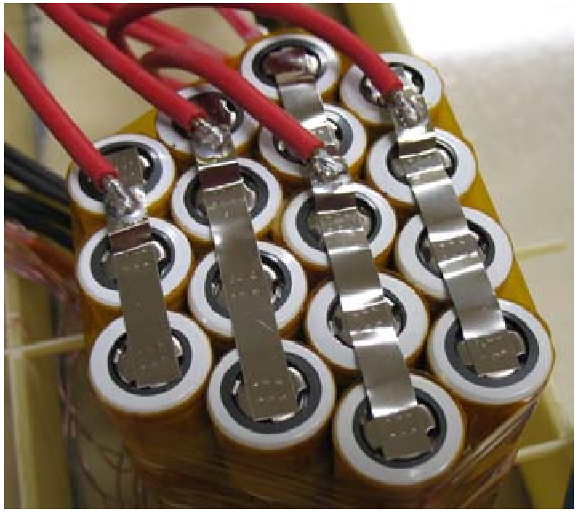


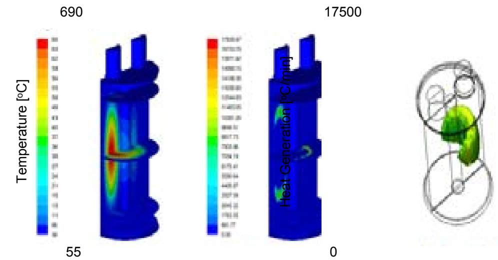
Photo: Symmetry Resources Inc. (SRI)

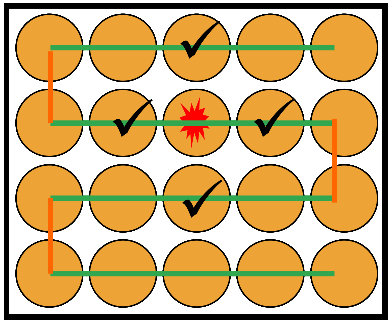
Modeling Approach

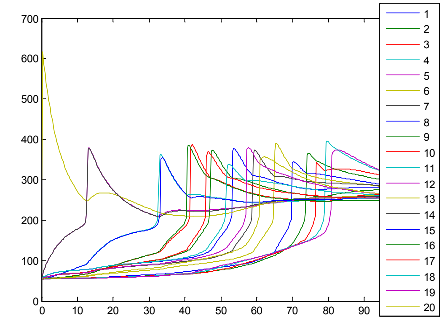
Previous Work:

- Design module to prevent thermal runaway propagation

Chemical Reaction Model + Thermal Network Model







Present Work:

- Verify module design tolerant to external electrical short

Electrical Model + Thermal Network Model

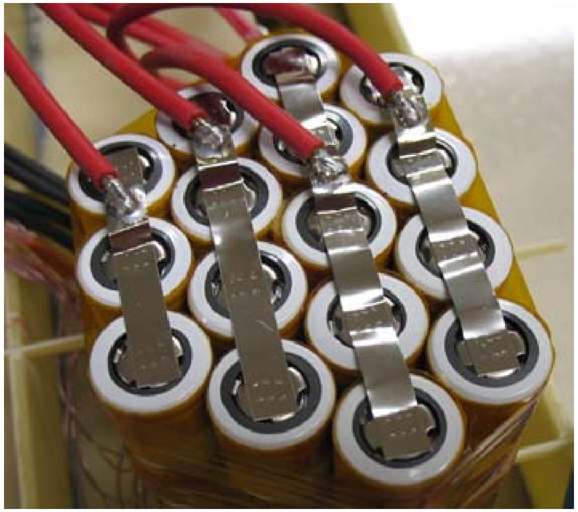
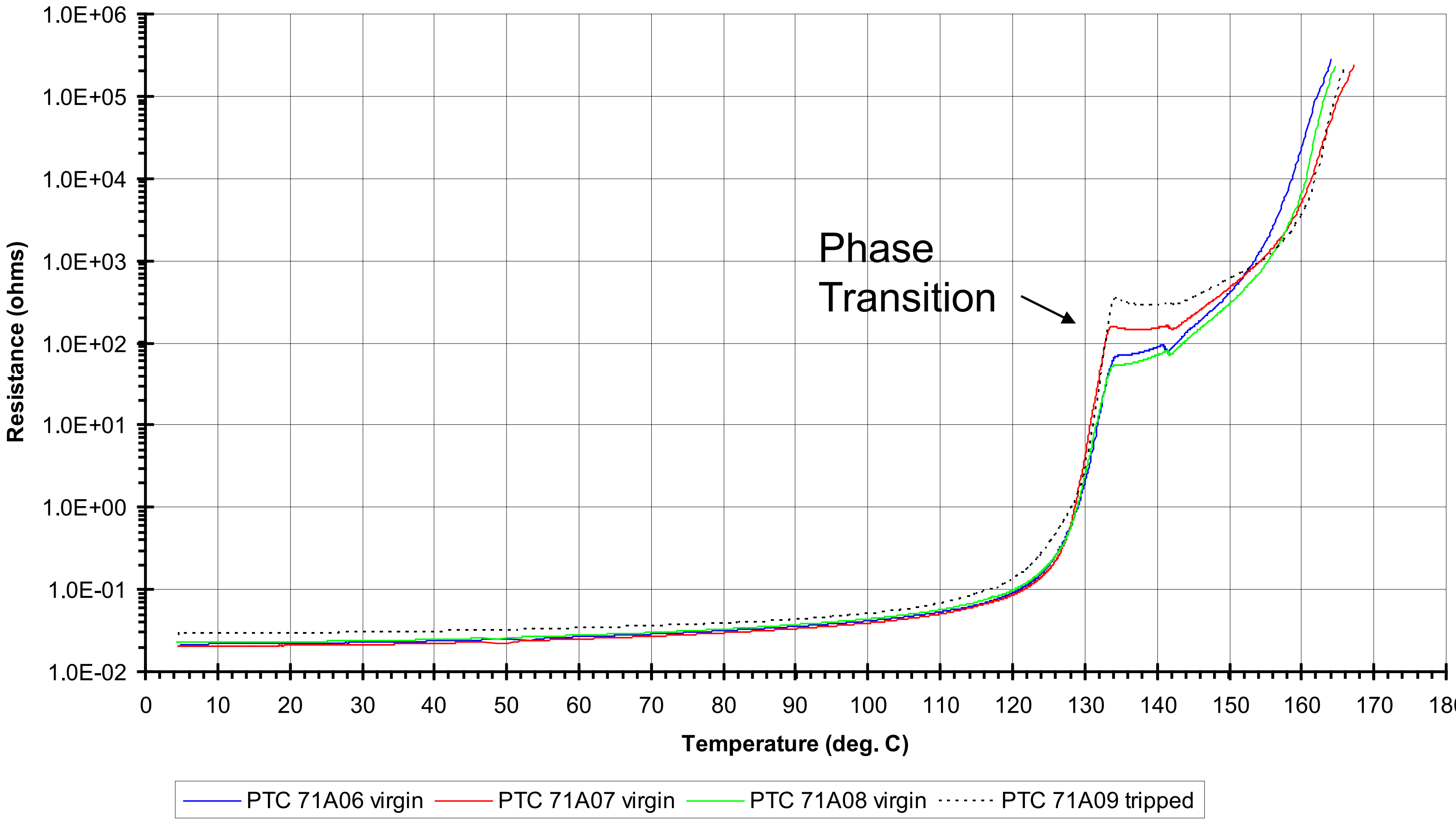


Photo: Symmetry Resources Inc.

PTC Resistance versus Temperature; Moli ICR-18650J

Cell header removed from cell without disturbing closure configuration
Resistance measurements taken from rupture disk surface to positive button



Behavior Principles of PTC Devices

Cell can be in 40°C range with two possible PTC device states

- Low-resistance current conducting state (<50 mΩ)
- Current-limiting state with high resistance (>1 kΩ)

Minimum and maximum base resistance (given ambient T)

- Minimum is for virgin (never been tripped) devices
- Maximum is for once (or more) tripped devices

Ultimate trip current, I_u, is the highest equilibrium current possible in the low-resistance state of the device for a given temperature

- It's the maximum current achieved in an I vs. V curve for a given ambient temperature, for example, at 45°C
  - Moli J's I_u = 7 A
  - LV's I_u = 9 A

Power generated in device = power dissipated in device

- The trip time depends on size of the overcurrent, ambient T, thermal mass of the device, its specific heat, its heat dissipation coefficient, and its base resistance
- Steady-state trip current is inversely proportional to voltage applied and ambient temperature

Model needs to capture important physics happening during an experiment

<u>*16P Bundle External Short Test*</u>

- *Performed by Symmetry Resources, Inc.*
- *Moli ICR18650J cells*
- *16 parallel*
- *10 mΩ external short*

Photos: SRI

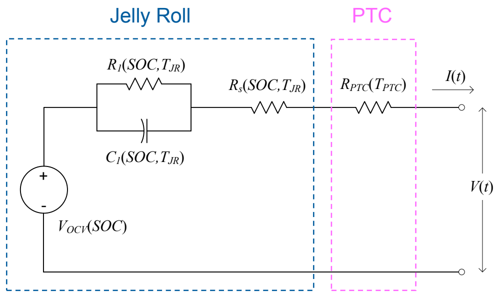
- PTC device behavior
  - $R_{PTC}(T)$
  - Thermal connection with the cell
- Cell electrical behavior
  - Current/voltage/temperature relationship
- Cell-to-cell heat transfer
  - Conduction
    - air gaps
    - electrical tabs
  - Radiation
- Cell-to-ambient heat transfer
  - Convection to air
  - Conduction through wire leads

Model Development Approach

***Integrated Thermal and Electrical Network Model** of a Multi-Cell Battery for Safety Evaluation of Module Design with PTC Devices during External Short*

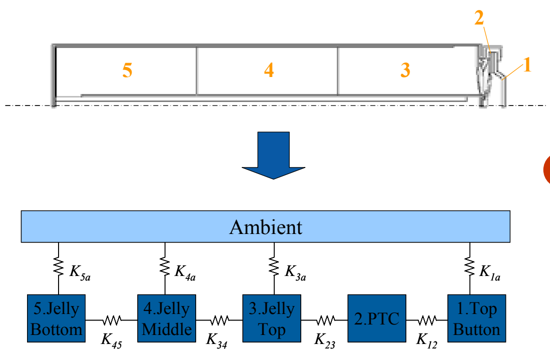
Unit Cell Model

Electrical Performance Model



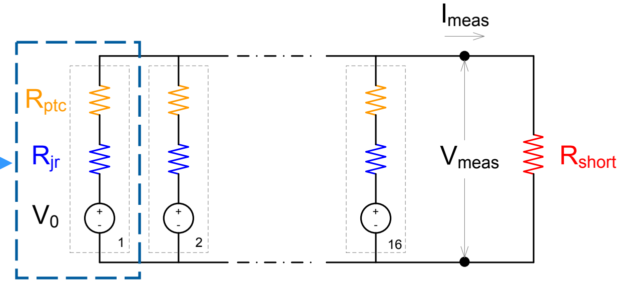
electrical/thermal interaction

5-Node Thermal Model



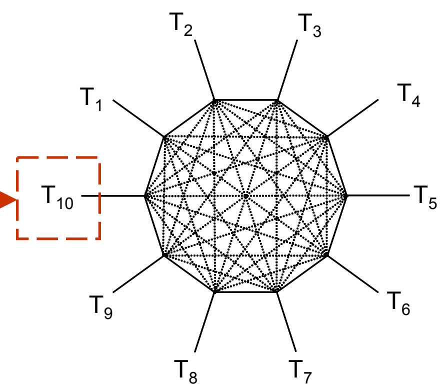
Multi-Cell T&E Network Model

Electrical Network Model

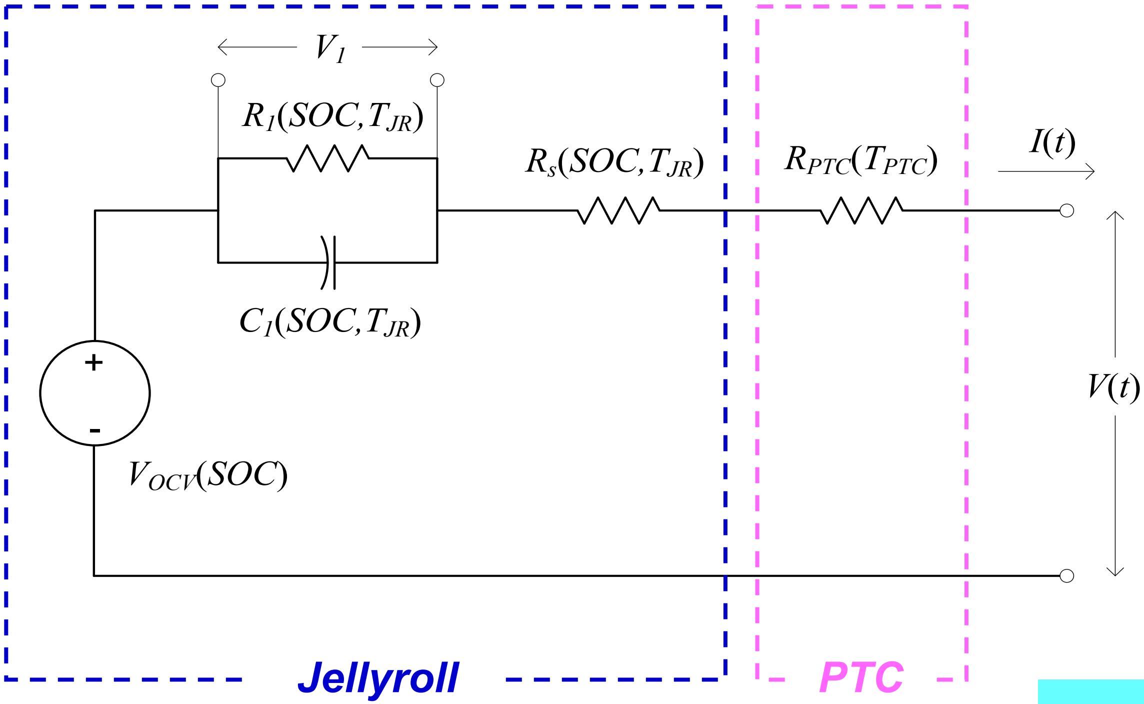


electrical/thermal interaction

Thermal Network Model



Unit Cell Model: Electrical Performance Model



Equivalent Circuit Model and Relevant Parameters

$$\lambda_1 = \frac{-1}{R_1 C_1}$$

$$Q = 2.345 \text{ A-h}$$

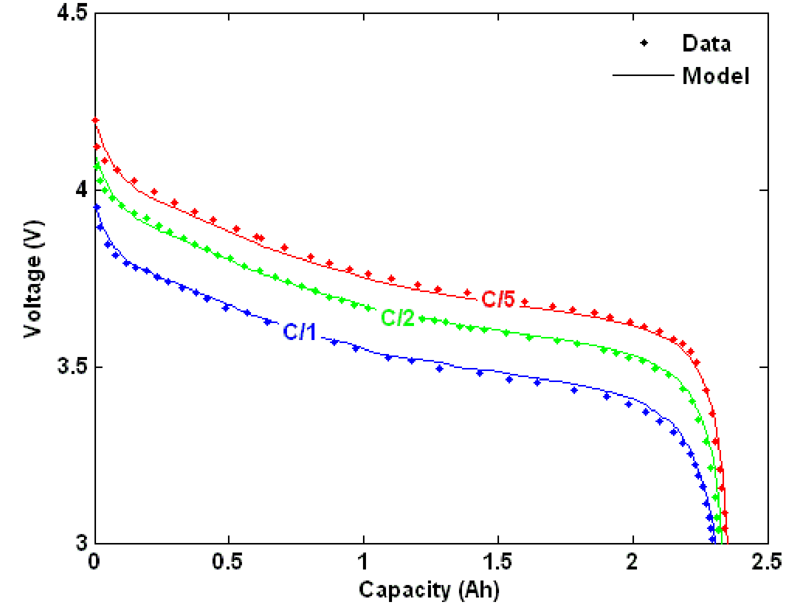
$$\frac{d}{dt}\begin{bmatrix} SOC \\ V_1 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & \lambda_1 \end{bmatrix}\begin{bmatrix} SOC \\ V_1 \end{bmatrix} + \begin{bmatrix} 1/Q \\ \lambda_1 R_1 \end{bmatrix} I(t)$$

$$V(t) = V_{OCV}(SOC) + V_1 - (R_s + R_{PTC}) \times I(t)$$

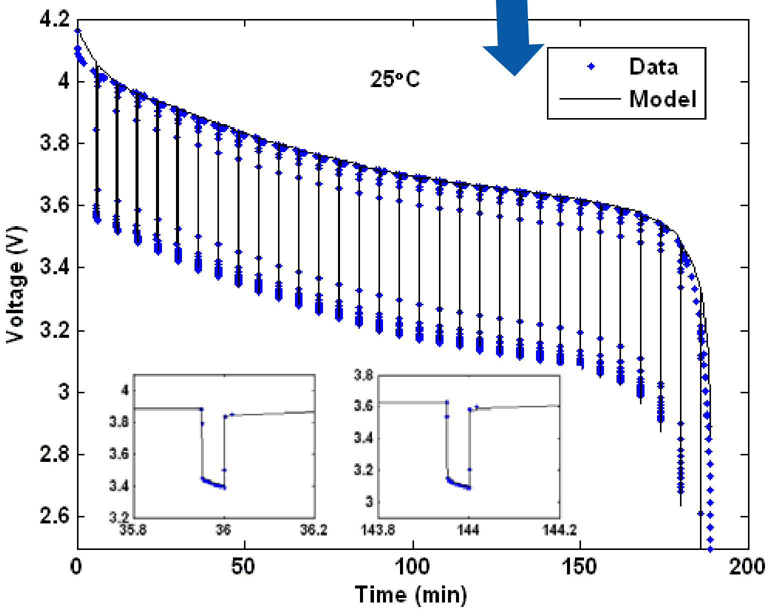
Unit Cell Electrical Model Agrees Well with Data

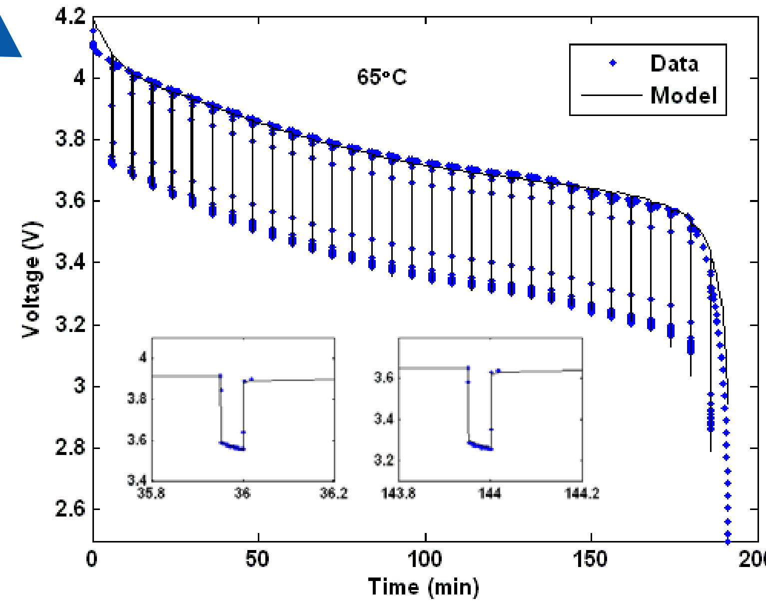
Validation of Equivalent Circuit Model

- Model compared with constant current discharge data from manufacturer (21C)



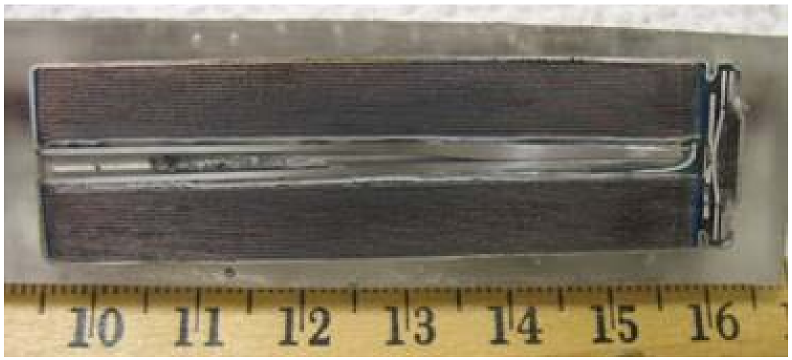
- Model compared with mission power profile data from NASA (25C and 65C)



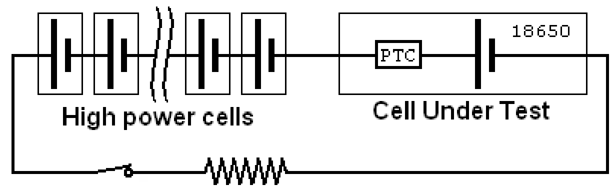


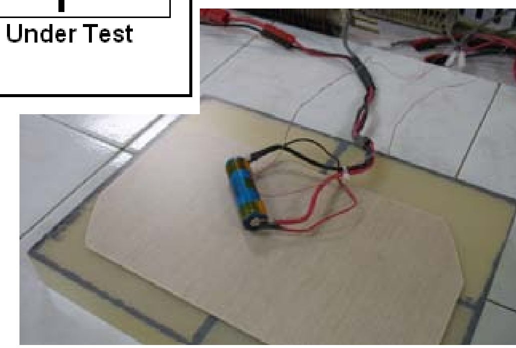
Unit Cell Model: Thermal Model

Developed detailed cell model based on cell cross-cut measurements…

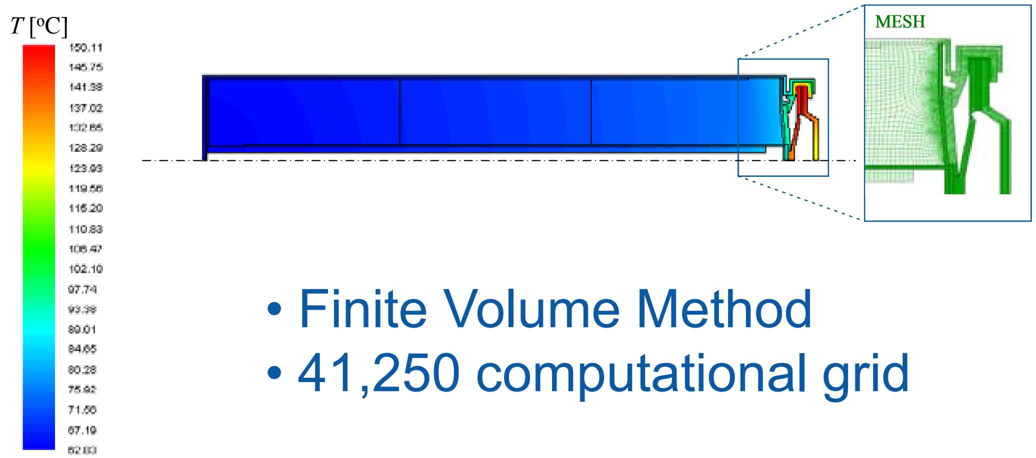


…and validated it with data from PTC device withstanding voltage test. (NASA/SRI)





Detailed Cell Thermal Model

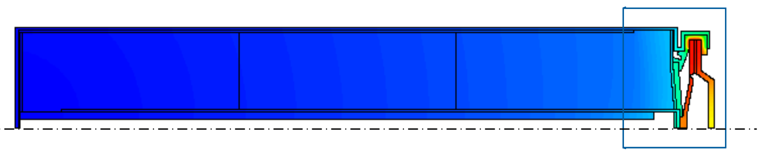


- Finite Volume Method
- 41,250 computational grid

Unit Cell Model: 5-nodeThermal Model Validated

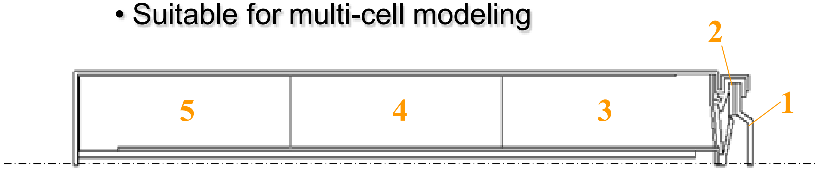
Detailed Cell Thermal Model

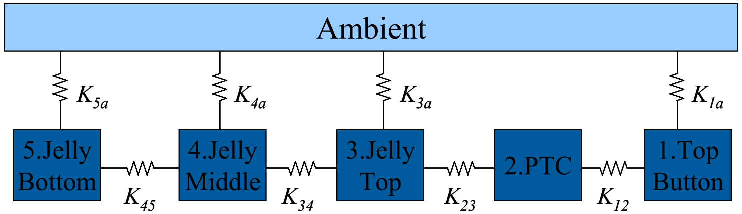
- Large computational requirement
- Not suitable for multi-cell modeling



5-Node Cell Thermal Model

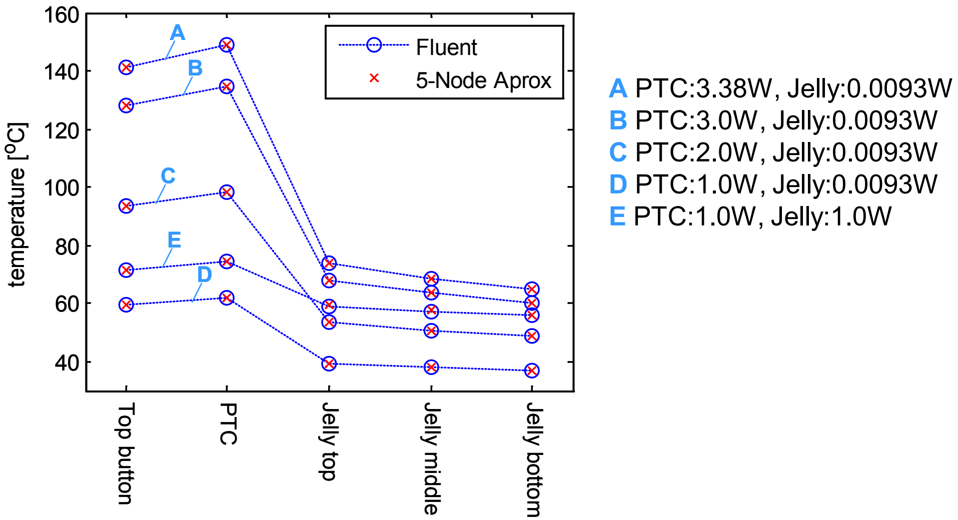
- Low order dynamic model
- Suitable for multi-cell modeling





Comparison of Detailed and 5–Node Models

For Different Heat Generation Conditions



Steady Form

$$Q_i = \sum_j K_{ij}\left(T_i - T_j\right)$$

Unsteady Form

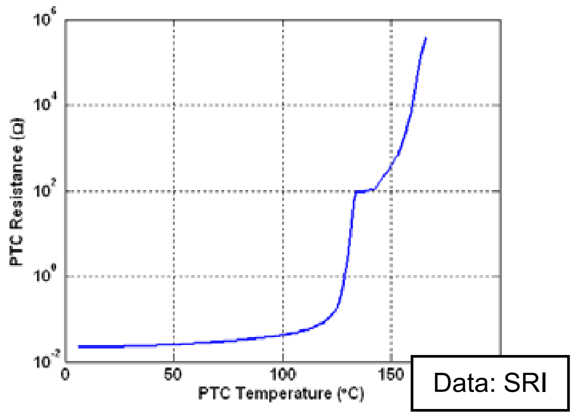
$$Q_i = \sum_j K_{ij}\left(T_i - T_j\right) + MCp_i \frac{dT_i}{dt}$$

Multi-Cell Network Model

Electrical Network Model

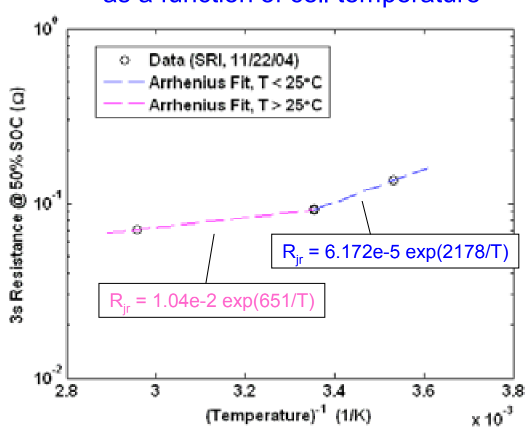
PTC Resistance

as a function of PTC temperature

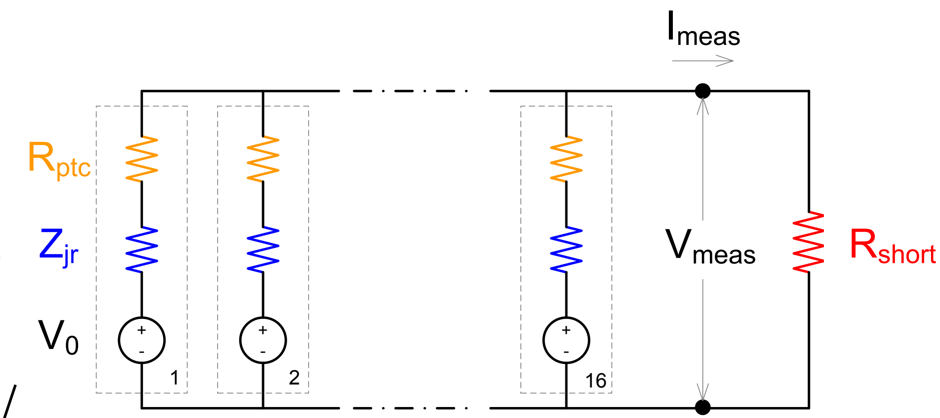


Jellyroll Resistance

as a function of cell temperature



The Model Solves Voltage and Current Interactions among the Components in a Multi-Cell Circuit



Open-Circuit Voltage

as a function of cell SOC

Multi-Cell Network Model

Thermal Network Model

Thermal Mass: Identifying thermal mass at each node
Heat Generation: PTC heat, charge transfer heat (future: abuse reaction heat)
Heat Transfer: Quantifying heat exchange among the nodes

$$Q_{transport,i} = \sum_{j=1, j\neq i} -Q_{ij}, \quad Q_{ij} = Q_{ij,radiation} + Q_{ij,connector\_conduction} + Q_{ij,convection} \cdots$$

Radiation Heat Transfer

Staggered Array

Let $X = 1 + \frac{d}{D}$

For $0 \le \frac{d}{D} \le \frac{2}{\sqrt{3}} - 1$, i.e. $1 \le X \le \frac{2}{\sqrt{3}}$

$$F_1 = \frac{1}{\pi}\left[-\sqrt{X^2-1} + \cos^{-1}\left(\frac{1}{X}\right) + \frac{\pi}{6}\right]$$

$$F_2 = \frac{1}{\pi}\left[\sqrt{X^2-1} - \cos^{-1}\left(\frac{1}{X}\right)\right]$$

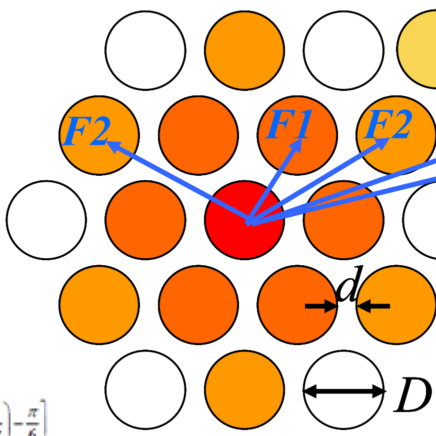
$$F_n = 0$$

For $\frac{2}{\sqrt{3}} - 1 < \frac{d}{D} \le 1$, i.e. $\frac{2}{\sqrt{3}} < X \le 2$

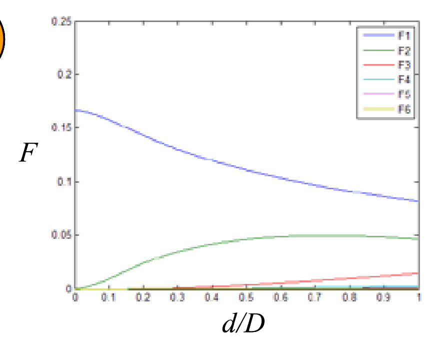
$$F_1 = \frac{1}{\pi}\left[\sqrt{X^2-1} - \cos^{-1}\left(\frac{1}{X}\right) - X + \frac{\pi}{2}\right]$$

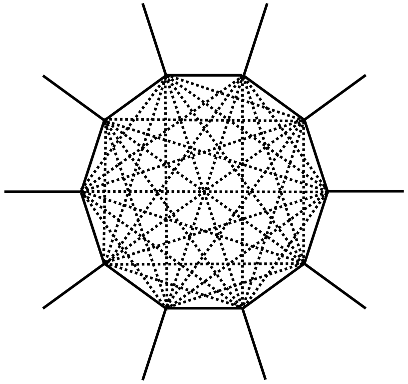
$$F_2 = \frac{1}{\pi}\left[\sqrt{3X^2-1} - 2\sqrt{X^2-1} + 2\cos^{-1}\left(\frac{1}{X}\right) - \cos^{-1}\left(\frac{1}{\sqrt{3}X}\right) - \frac{\pi}{6}\right]$$

$$F_n = \frac{1}{2\pi}\left[\begin{array}{l} \sqrt{\{n(n-1)+1\}X^2-1} - 2\sqrt{\{(n-1)(n-2)+1\}X^2-1} + \sqrt{\{(n-2)(n-3)+1\}X^2-1} \\ -\cos^{-1}\left(\frac{1}{\sqrt{n(n-1)+1}X}\right) + 2\cos^{-1}\left(\frac{1}{\sqrt{(n-1)(n-2)+1}X}\right) - \cos^{-1}\left(\frac{1}{\sqrt{(n-2)(n-3)+1}X}\right) \\ +\tan^{-1}\left\{\frac{2}{\sqrt{3}}\left(n-\frac{1}{2}\right)\right\} - 2\tan^{-1}\left\{\frac{2}{\sqrt{3}}\left(n-\frac{3}{2}\right)\right\} + \tan^{-1}\left\{\frac{2}{\sqrt{3}}\left(n-\frac{5}{2}\right)\right\} \end{array}\right]$$



$$Q_{ij,radiation} = \varepsilon F_{ij} A (T_i^{\,4} - T_j^{\,4})$$





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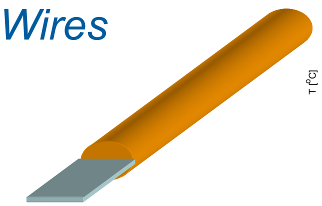
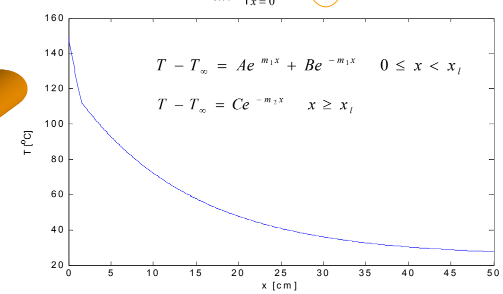
Heat Transfer to Ambient

$$Q_{i-a} = hA_{i-a}(T_i - T_\infty)$$

Heat Rejection Through Wires

$$Q_{base} = kA_b \left.\frac{dT}{dx}\right|_{x=0} = hA(T_b - T_\infty)$$

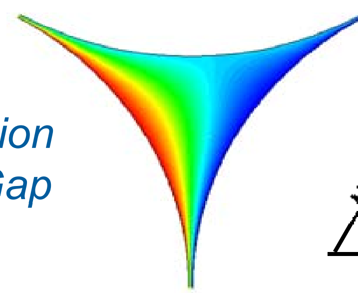


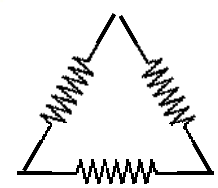


Conduction Through Bus

$$R_{connector,i-j} = \frac{L_{i-j}}{k_{i-j} A_{i-j}}$$

Heat Conduction Through Air-Gap

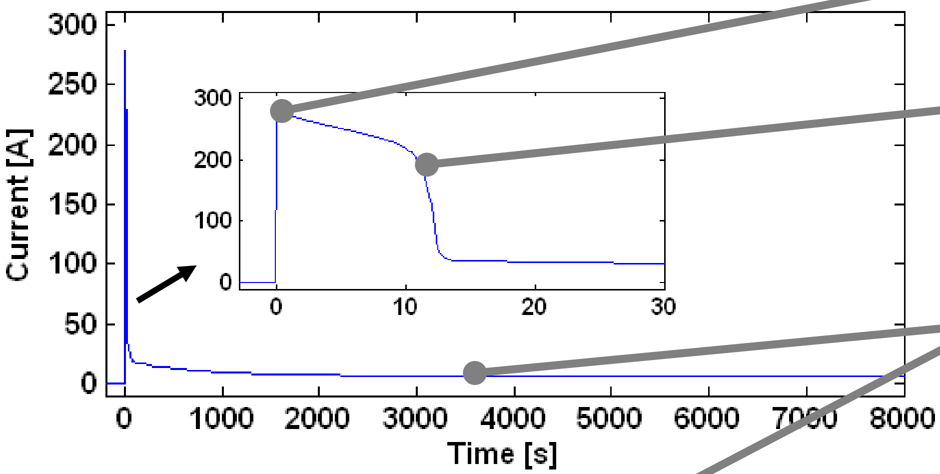


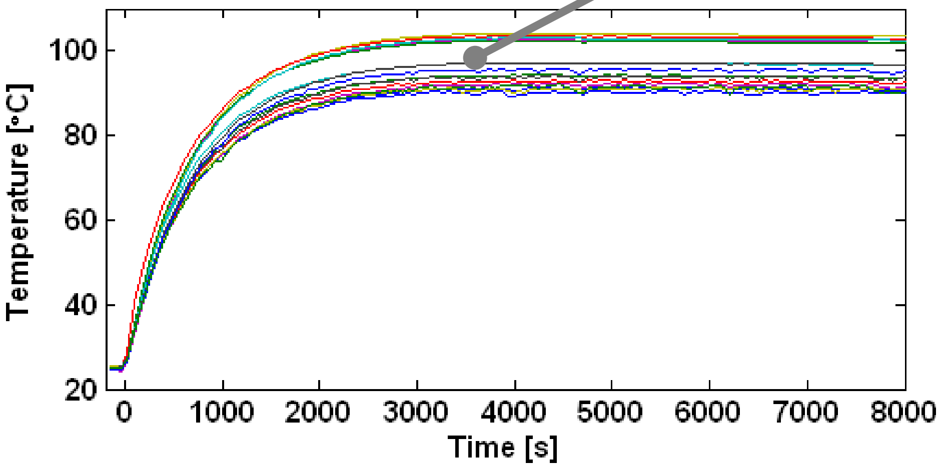


Experimental Model Validation

10 mΩ External Short

Data & Photo: SRI

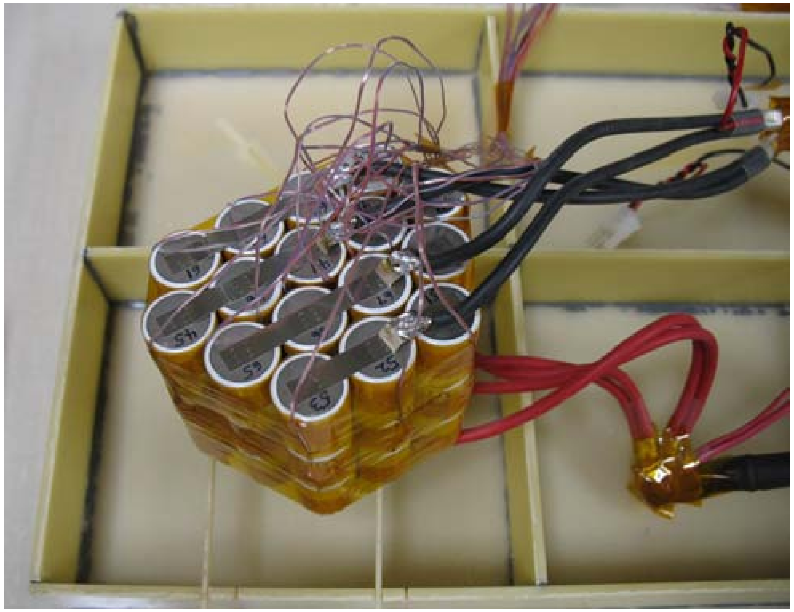




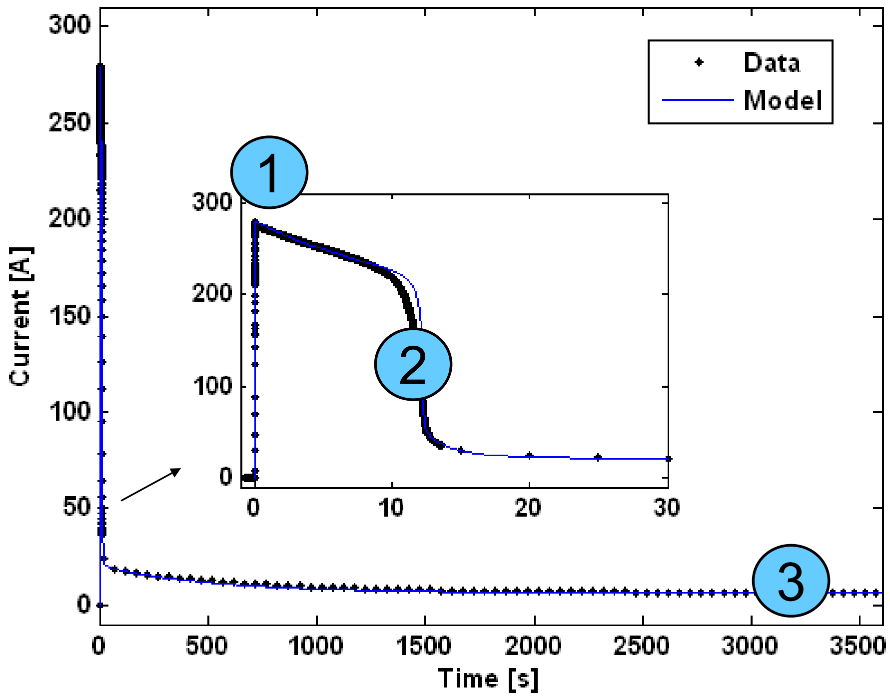
1) t = 0 sec: Circuit closed

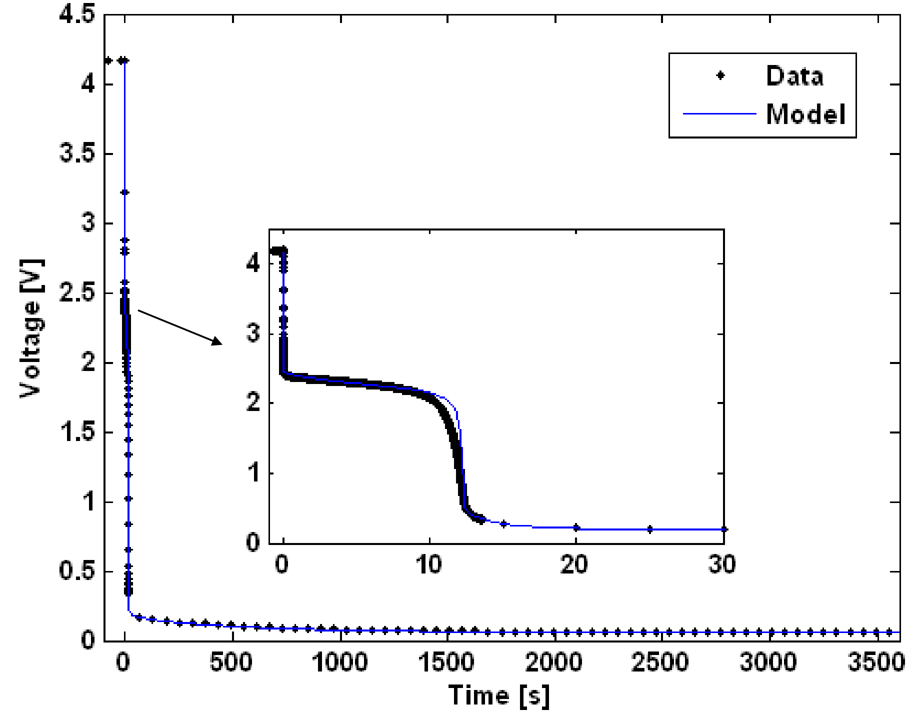
2) t ≈ 12 sec: PTC devices trip
   - $T_{PTC} \approx 130°C$

3) t ≈ 1 hr: Steady state reached
   ~ C/5 discharge



Model Validation – Current & Voltage





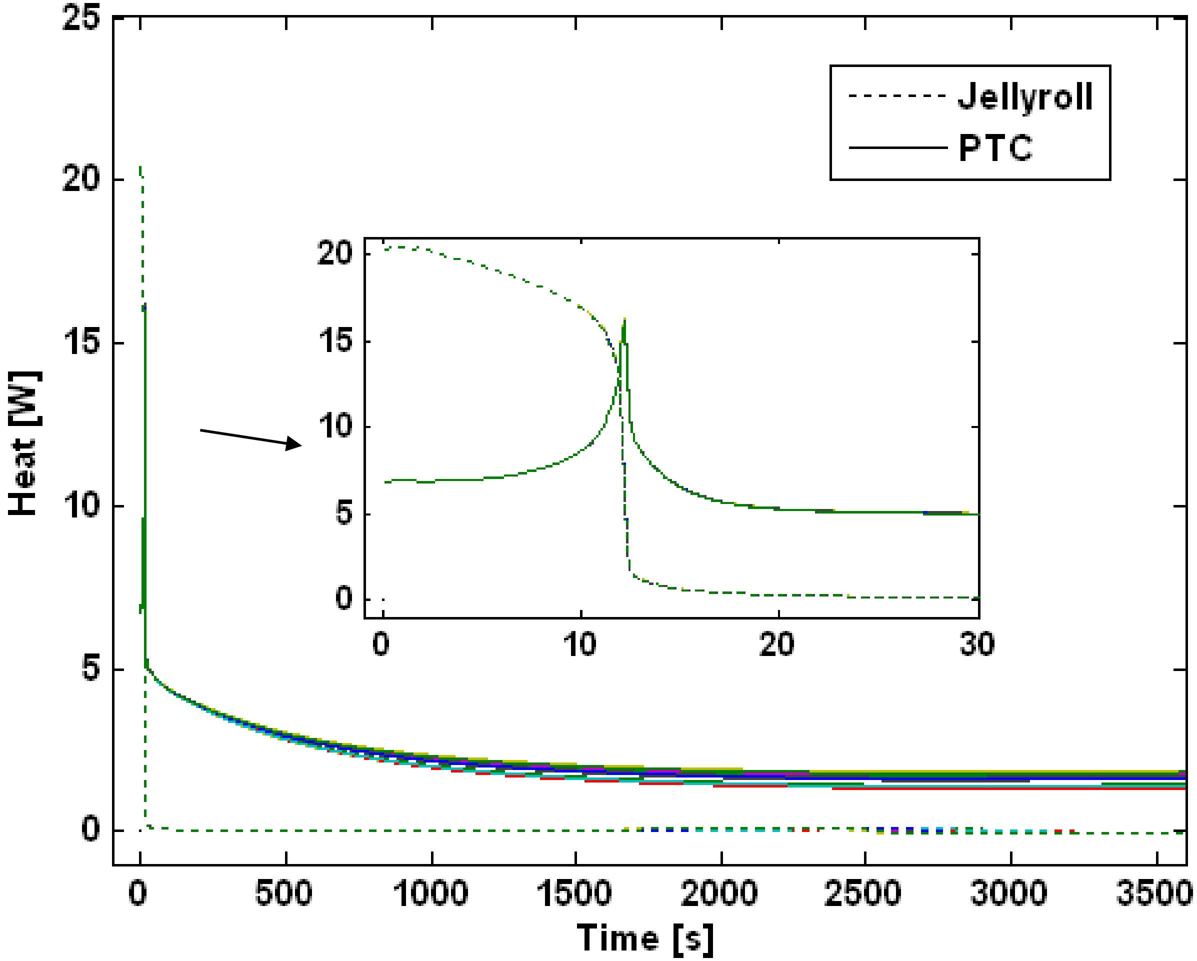
1. Peak inrush current readily predicted with knowledge of cell & short resistances.

2. PTC device trip time affected by
   - PTC thermal mass
   - PTC conductive path to jellyroll & can.

3. Steady-state behavior affected by jellyroll and PTC device temperature, indirectly
   - PTC conductive path to jellyroll & can
   - Thermal boundary conditions to ambient.

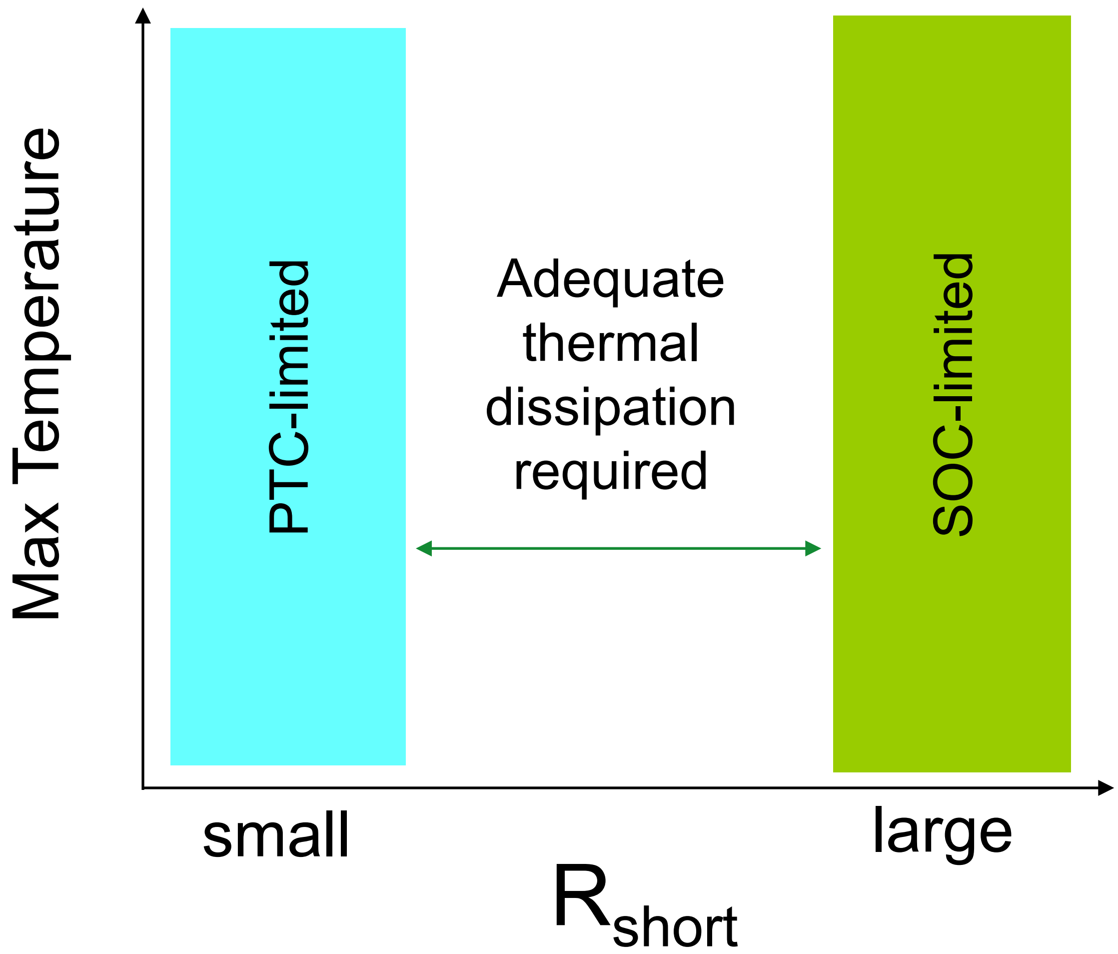
Model Prediction – Heat Generation

- Pre-trip: Jellyroll heat generation dominates.
- Post-trip: PTC device heat generation dominates.

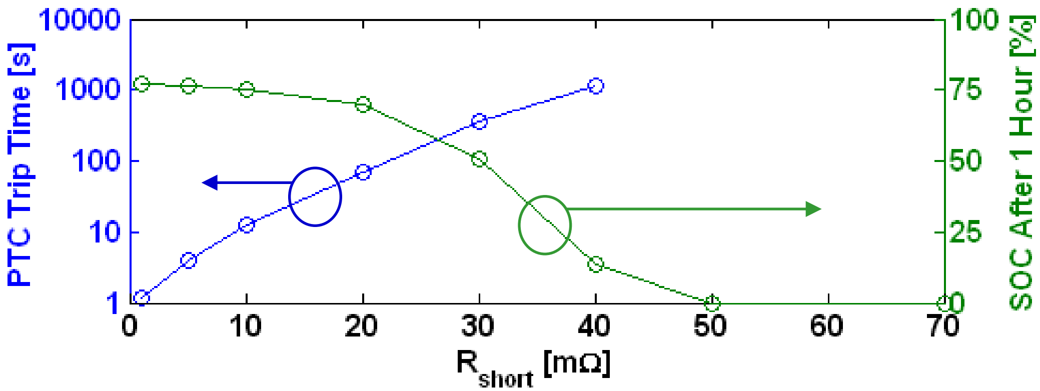


PTC devices at steady-state 1.35 to 1.86 W

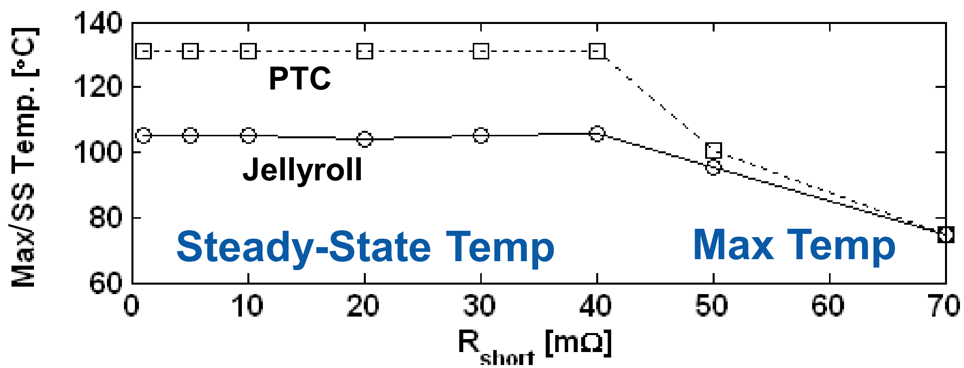
Is this design safe under other short conditions?



Simulation Results at Various Values of R_{short}



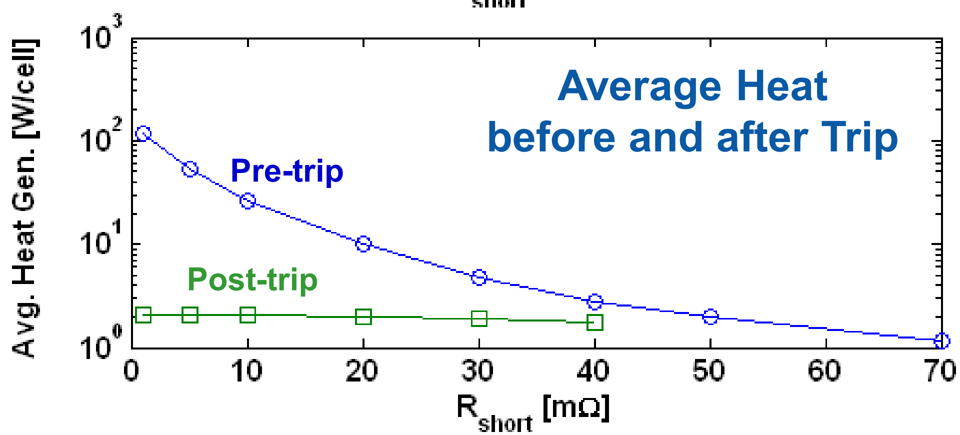
- R_{short} ≤ 40 mΩ: PTC-limited
- R_{short} ≥ 50 mΩ: SOC-limited



- Tripped PTC device serves as thermal regulator

  $[dR_{PTC}/dT]_{130^\circ C} = 3\Omega/^\circ C$

  (5 orders of magnitude > than at 25˚C)



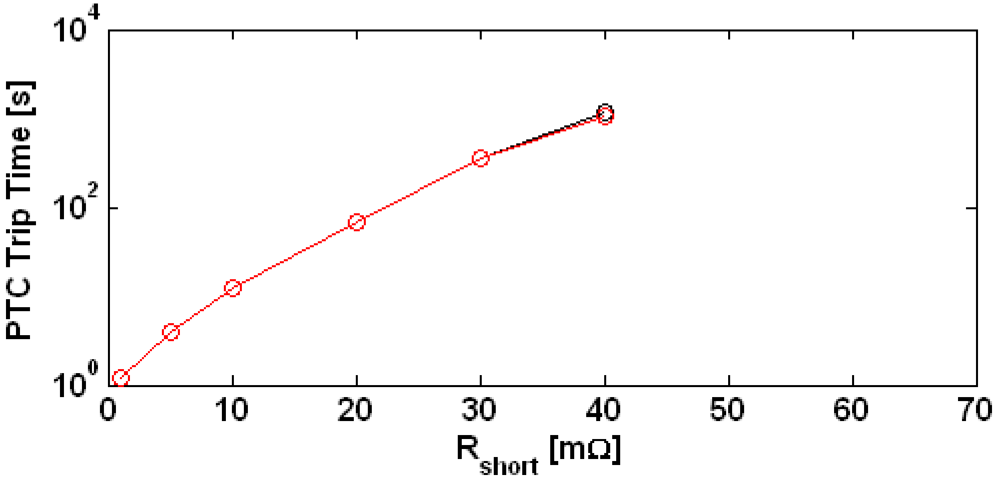
- Large pre-trip heat rates are safe provided they are of
  - short duration
  - sufficient thermal mass
  - sufficient heat dissipation

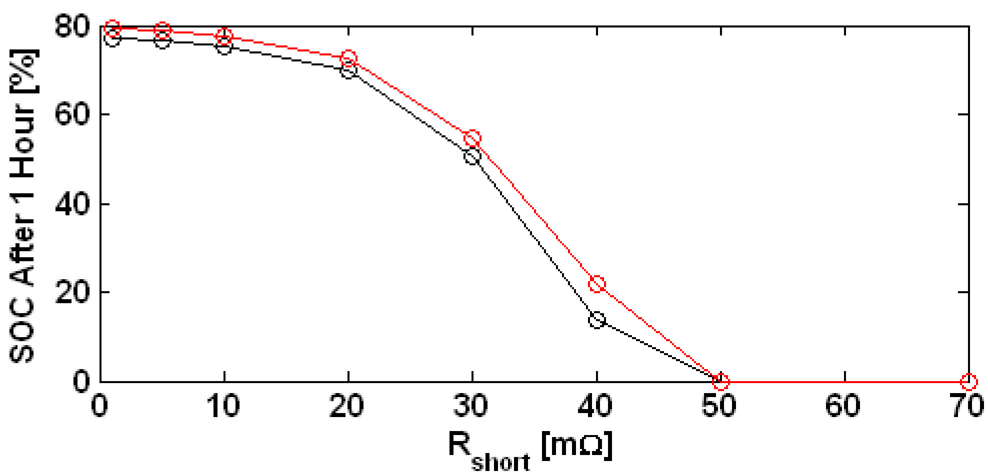
How much heat rejection is required for safety?

Additional simulations run with various values of h (convective heat transfer coefficient to ambient).

Red lines: $h = h_{nominal} / 2$

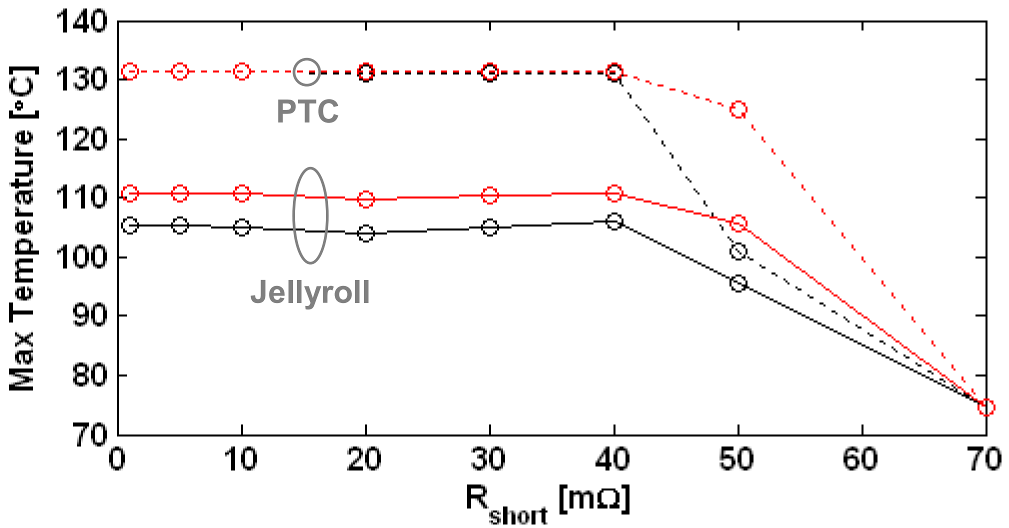
Black lines: $h = h_{nominal}$

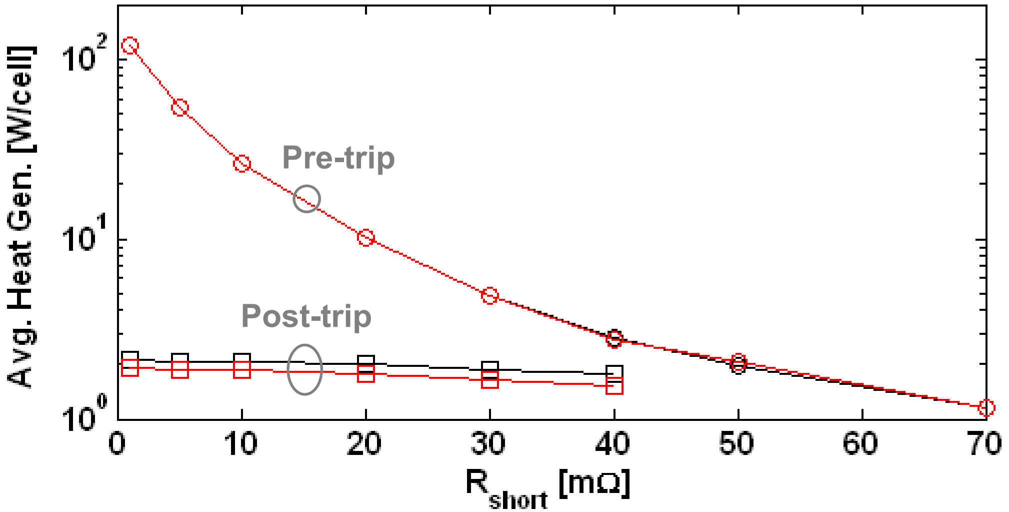




- PTC device trip time decreases only slightly with less heat rejection from cells.
- Less rejection leads to hotter PTC device (higher resistance) and slower discharge of cell.

How much heat rejection is required for safety?





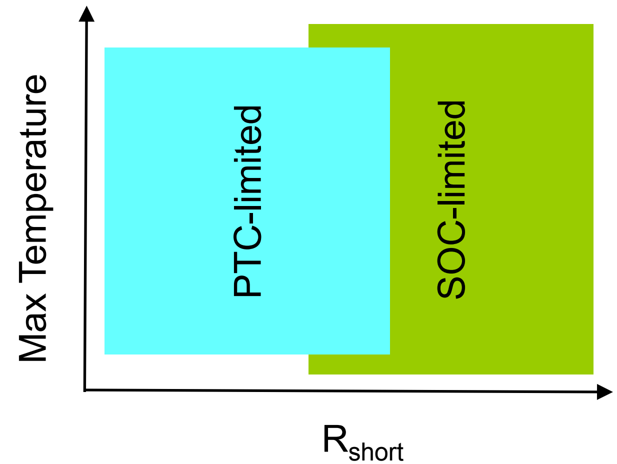
Red lines: $h = h_{nominal} / 2$

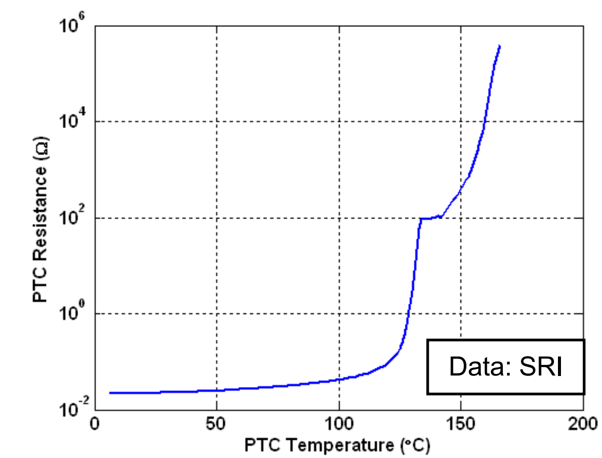
Black lines: $h = h_{nominal}$

- Less rejection causes an increase in jellyroll temperature.
- Pre-trip heat generation rate is largely unaffected by thermal boundary conditions.
- Post-trip, the PTC device reduces heat generation rate as heat rejection decreases.

Conclusions

- Created & validated a new multi-cell math model capturing electrical and thermal interactions of cells with PTC devices during abuse. Suitable for
  - Assessing battery safety design margins
  - Supplementing and guiding verification tests
- Moli ICR18650J cell design has promise to be tolerant to a wide range of external shorts for the 16p configuration of a spacesuit battery, as long as
  - No damage occurs due to the in-rush current transient
  - Nominal tripping of cell PTC devices and steady-state conditions occur
  - External short does not excessively heat battery.
- PTC device is an effective thermal regulator. Maximum cell temperature (final state) is very similar for a variety of initial and boundary conditions.





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