National Renewable Energy Laboratory
Innovation for Our Energy Future

Thermal/Electrical Modeling for Abuse-Tolerant Design of Li-Ion Modules

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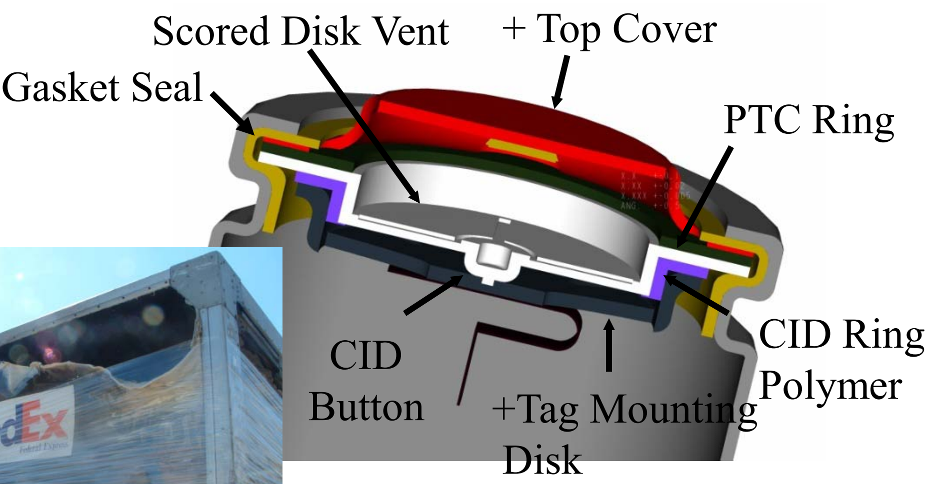
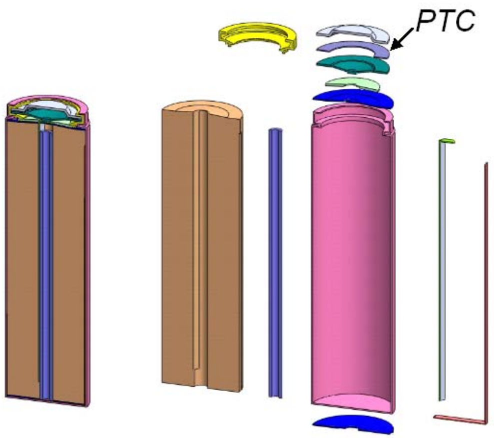
Background and Motivation for Present Work

- **Background**
  - Cell PTC device proven effective control for overcurrent hazards at Li-Ion cell and small battery level
  - Proven ineffective in high-voltage battery designs
  - Fire in 2004 Memphis FedEx facility suspected due to PTC device failures in large capacity (66p-2s) battery shorted while at 50% SOC
- **Motivation**
  - 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

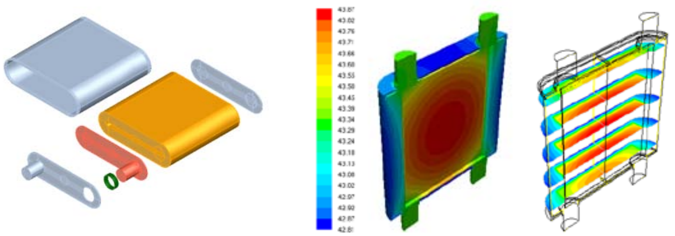


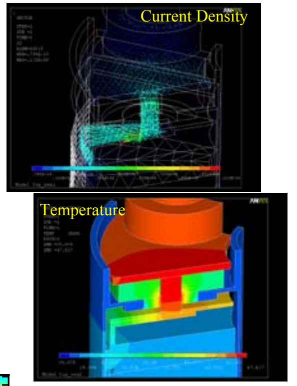
- Create an engineering model to guide the design and to verify safety margin of a battery using high specific energy COTS cells

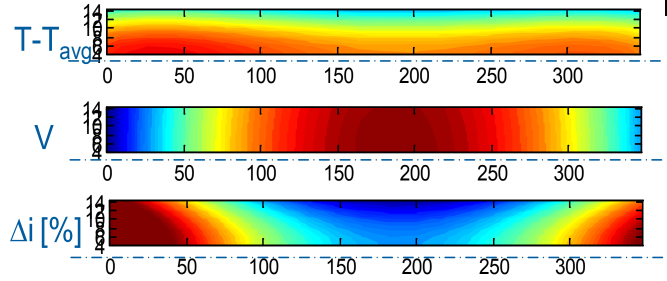
- Use the model to provide input for designing NASA 16p-5s 18650 spacesuit battery
  - Cell model must include the electrical and thermal behavior of the cell PTC device
  - Use cell model as building block to model multicell battery behavior under short-circuit conditions
  - Assess the range of smart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

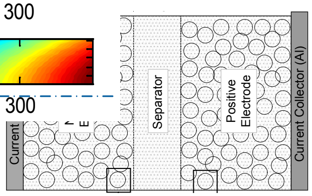
Utilizing NREL's Multiphysics Battery Modeling

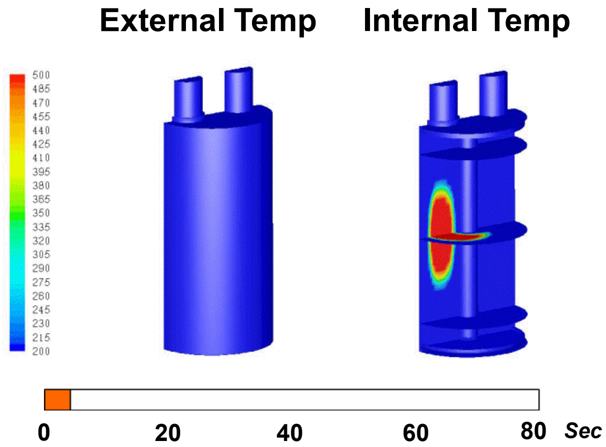
- Electrical Performance Modeling
  - Cells & multistring modules
- Thermal Modeling
  - Cells & modules
- Thermal/Electrochemical Modeling
  - Cells
- Thermal/Chemical Abuse Modeling*
  - Cells and modules

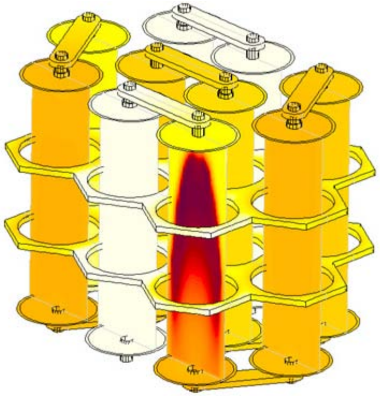


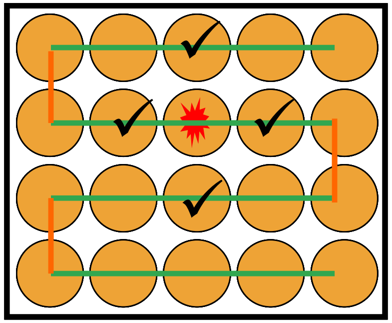








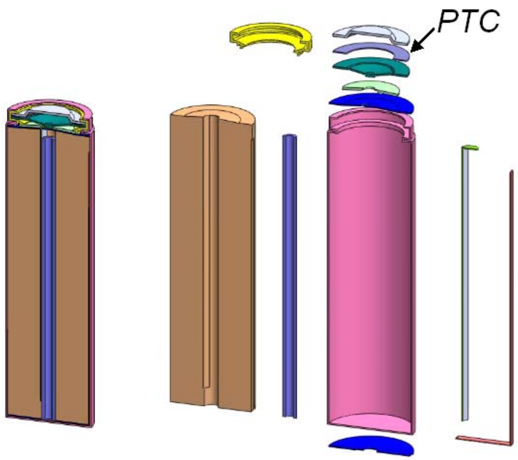




*G.-H. Kim, A. Pesaran, "Analysis of heat dissipation in Li-ion cells and modules for modeling of thermal runaway," 3rd International Symposium on Large Lithium Ion Battery Technology and Application, Long Beach, CA, May 2007. Available: www.nrel.gov/vehiclesandfuels/energystorage/

Overview

- Modeling
  - Approach
  - PTC device (discussed by Eric Darcy)
  - Cell
    - Electrical
    - Thermal (5-node)
  - Module
    - Electrical (multinode network)
    - Thermal (multinode 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



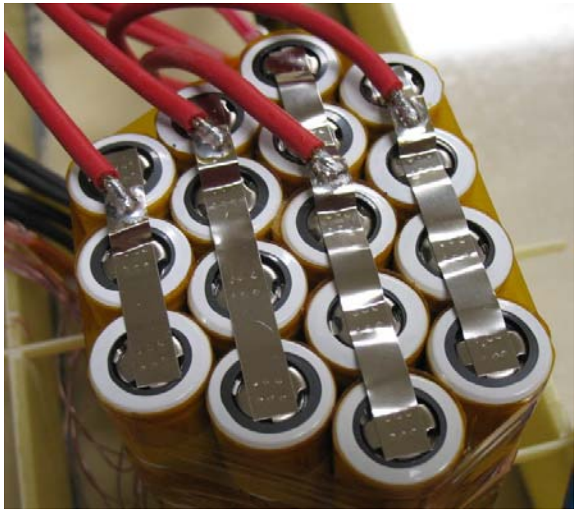


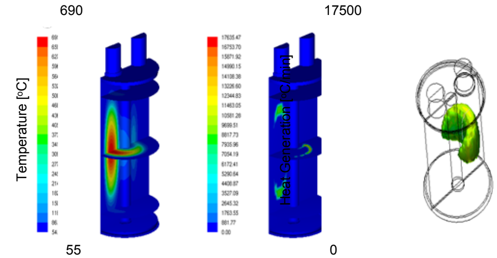
Photo: Symmetry Resources Inc. (SRI)

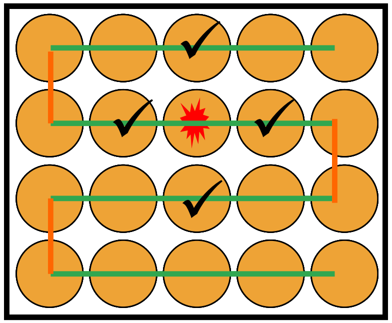
Modeling Approach

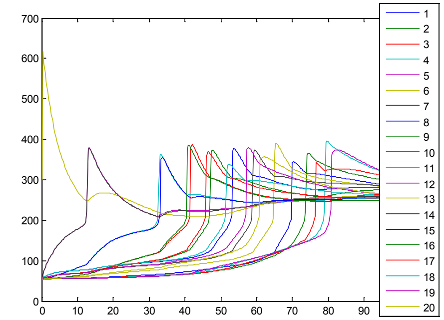
Previous Work:

- 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

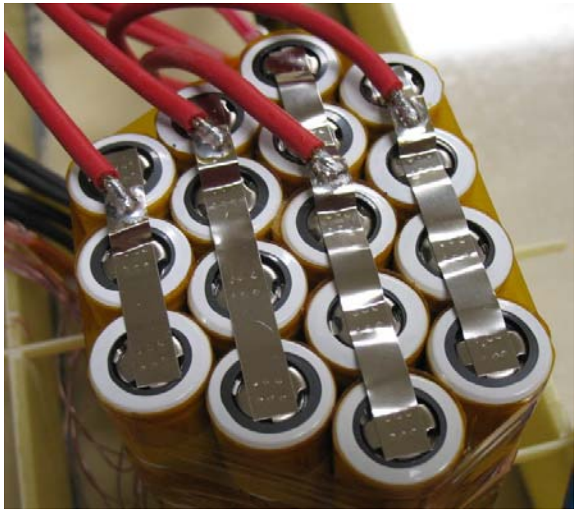
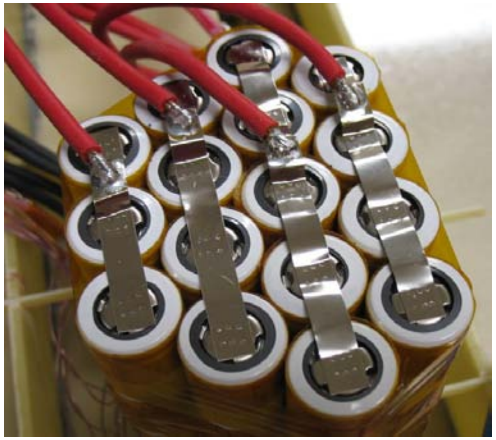


Photo: Symmetry Resources Inc.

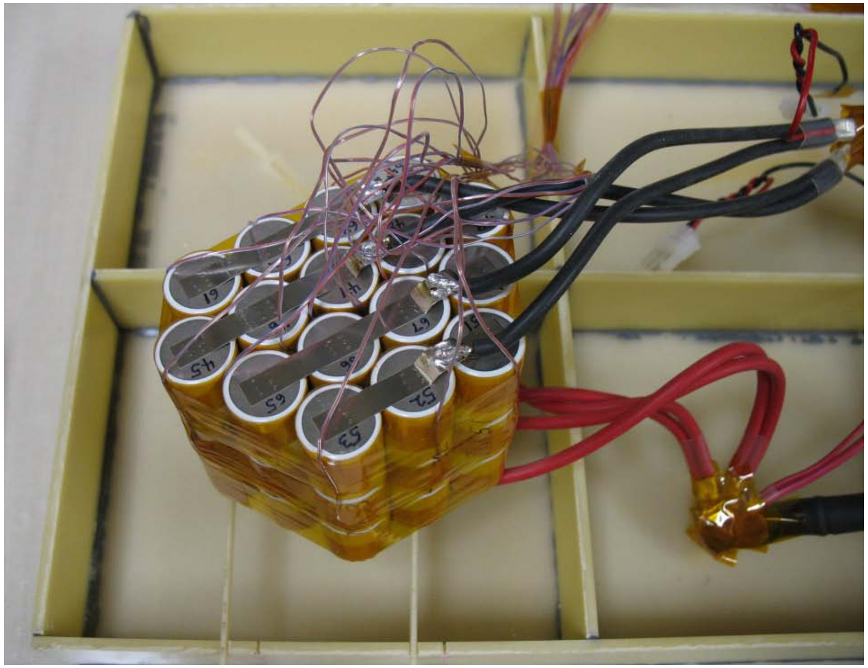
Model has to capture important physics happening during an experiment

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

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



Photos: SRI



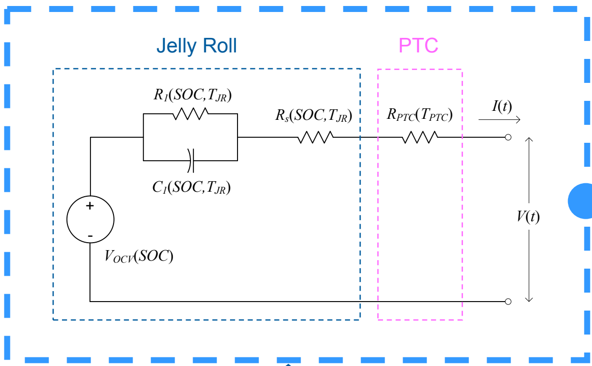
- PTC device behavior
  - $R_{PTC}(T)$
  - Thermal connection with the cell
- Cell electrical behavior
  - Current/voltage/temperature relationship
- Cell-to-cell heat transfer
  - Conduction
    - air gaps
    - electrical tabs
  - radiation
- Cell-to-ambient heat transfer
  - Convection to air
  -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

Model Development Approach

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

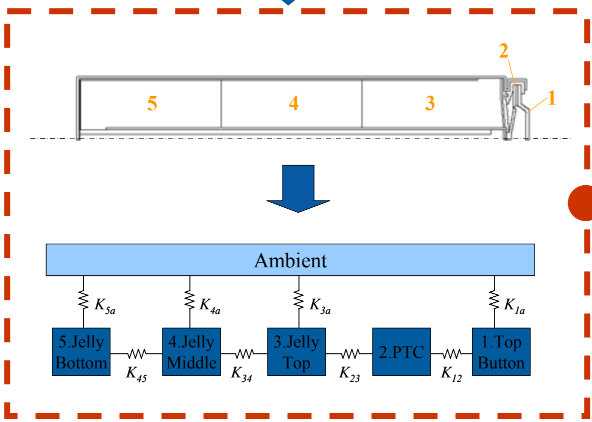
Unit Cell Model

Electrical Performance Model



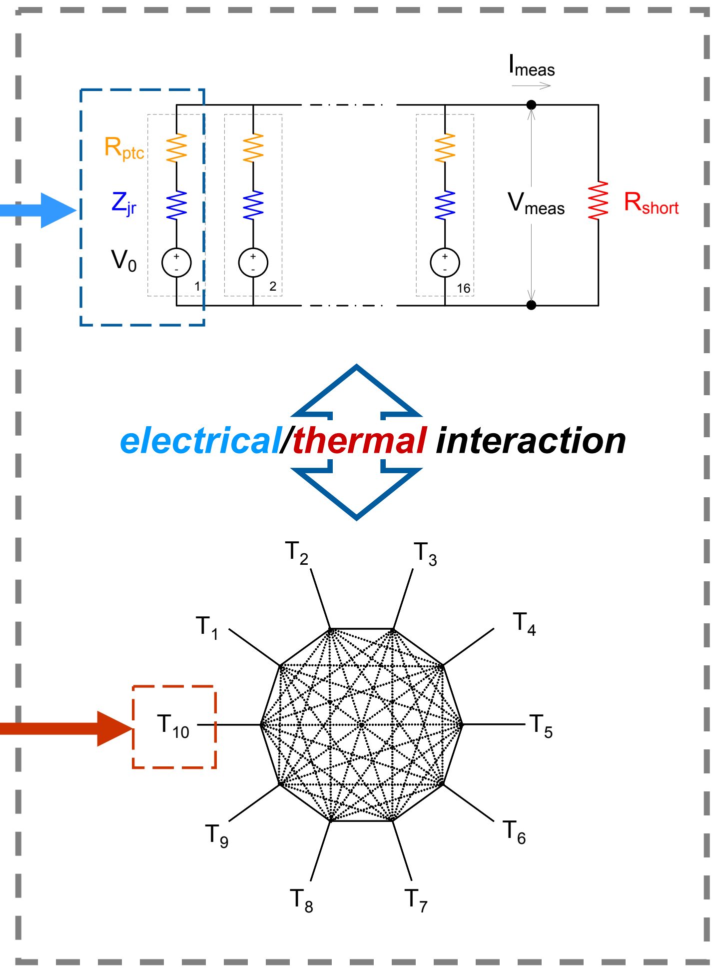
electrical/thermal interaction

5-Node Thermal Model



Multicell T&E Network Model

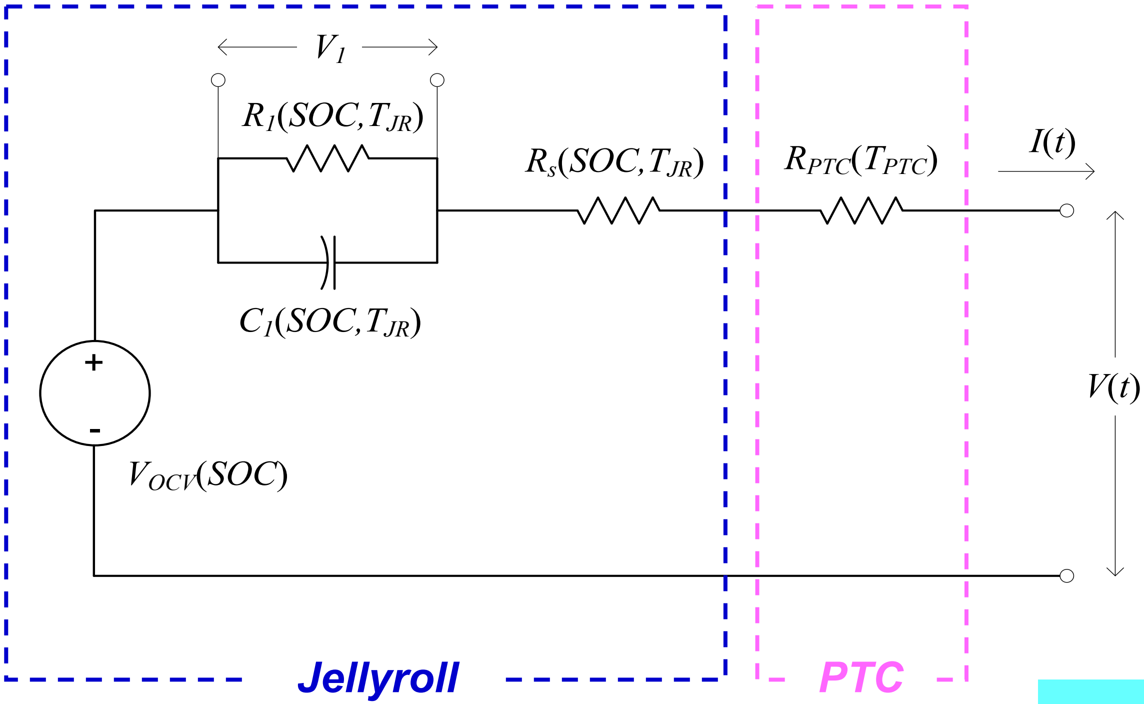
Electrical Network Model



electrical/thermal interaction

Thermal Network Model

Unit Cell Model: Electrical Performance Model



Equivalent Circuit Model and Relevant Parameters

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

$$Q = 2.345 \text{ Ah}$$

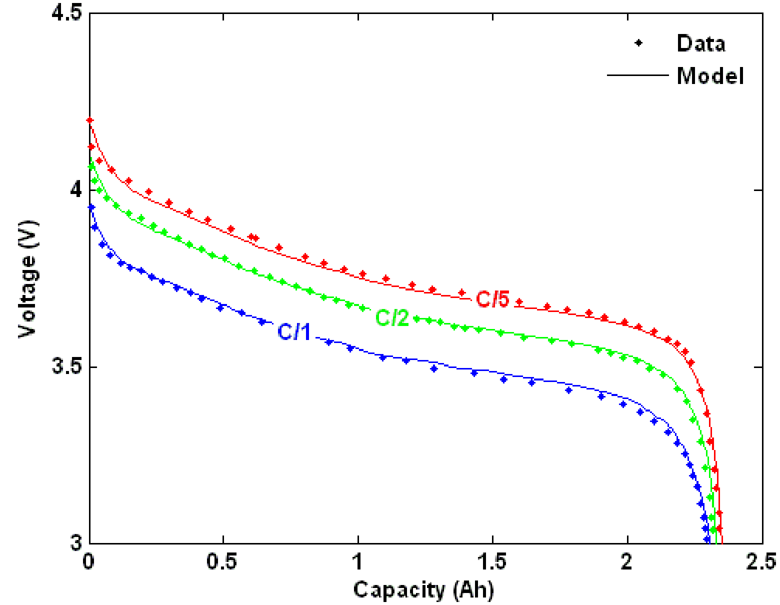
$$\frac{d}{dt}\begin{bmatrix} SOC \\ V_1 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & \lambda_1 \end{bmatrix}\begin{bmatrix} SOC \\ V_1 \end{bmatrix} + \begin{bmatrix} 1/Q \\ \lambda_1 R_1 \end{bmatrix} I(t)$$

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

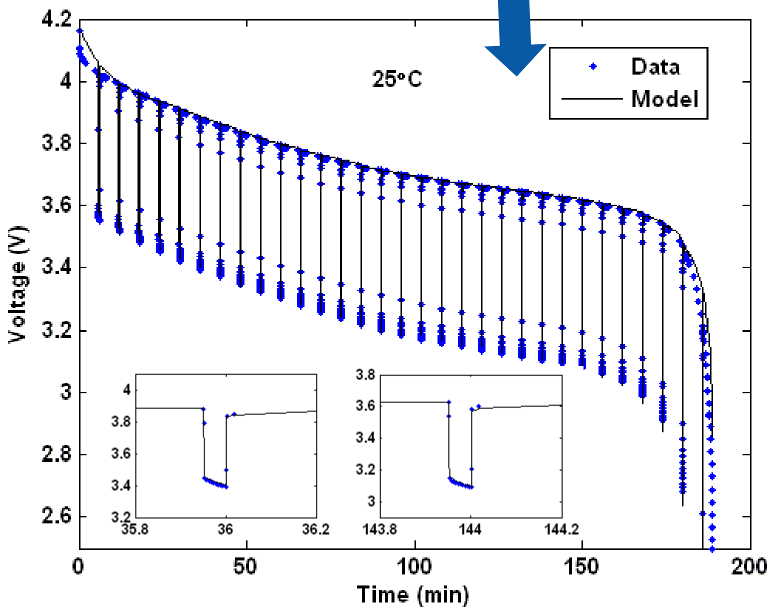
Unit Cell Electrical Model Agrees Well with Data

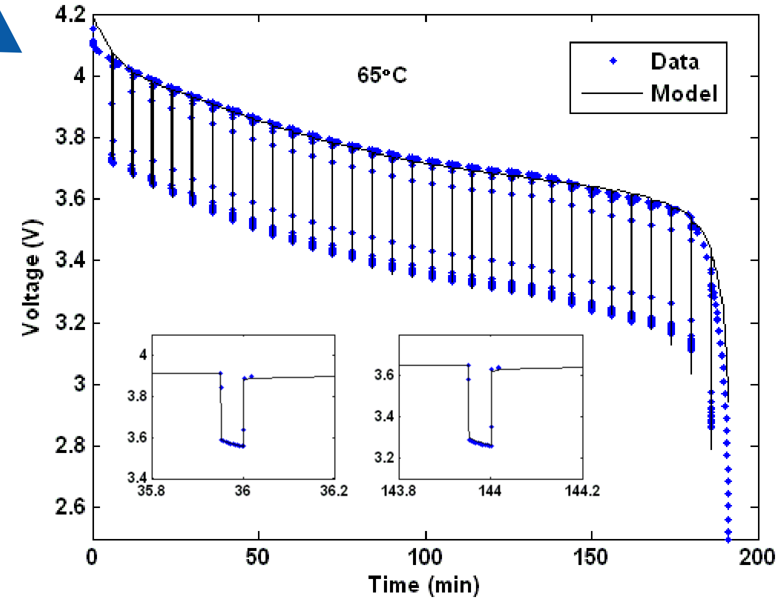
Validation of Equivalent Circuit Model

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



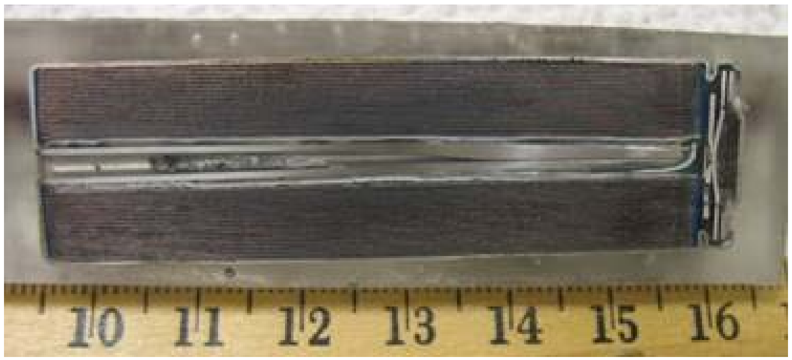
- Model results compared with mission power profile data from NASA (25C and 65C)



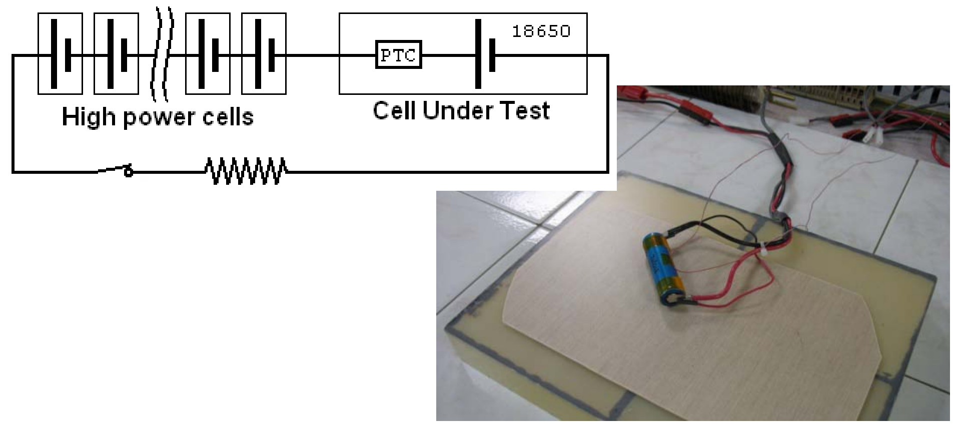


Unit Cell Model: Thermal Model

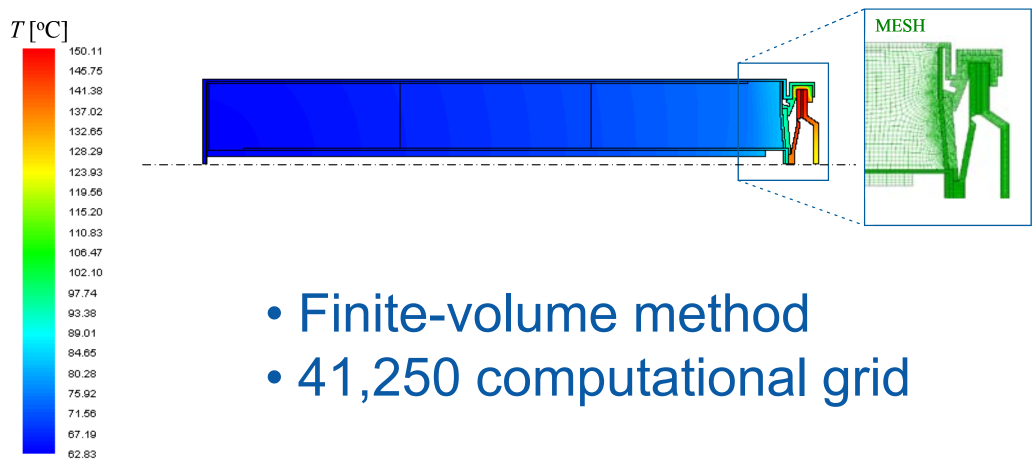
Developed detailed cell model based on cell cross-cut measurements…



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



Detailed Cell Thermal Model

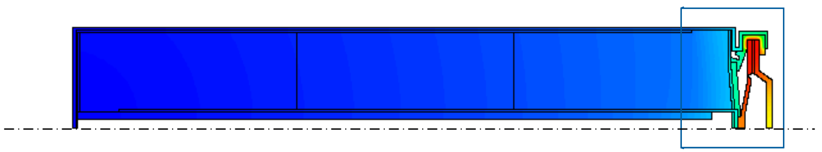


- Finite-volume method
- 41,250 computational grid

Unit Cell Model: 5-nodeThermal Model Validated

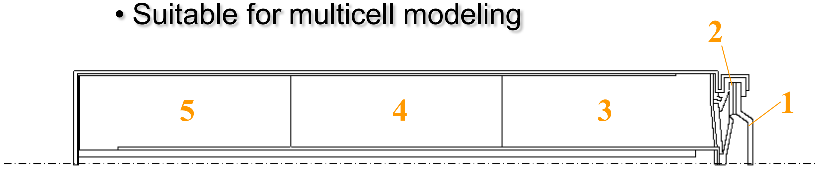
Detailed Cell Thermal Model

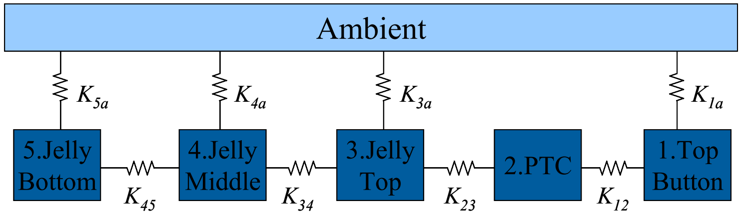
- Large computational requirement
- Not suitable for multicell modeling



5-Node Cell Thermal Model

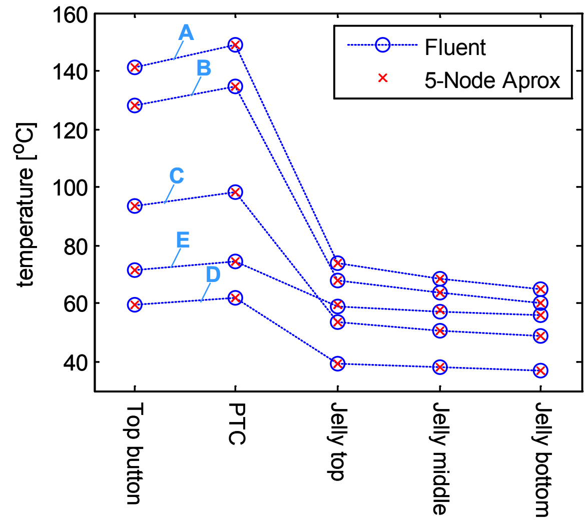
- Low order dynamic model
- Suitable for multicell modeling





Comparison of Detailed and 5-Node Models

for different heat generation conditions



A PTC:3.38W, Jelly:0.0093W
B PTC:3.0W, Jelly:0.0093W
C PTC:2.0W, Jelly:0.0093W
D PTC:1.0W, Jelly:0.0093W
E PTC:1.0W, Jelly:1.0W

Steady Form

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

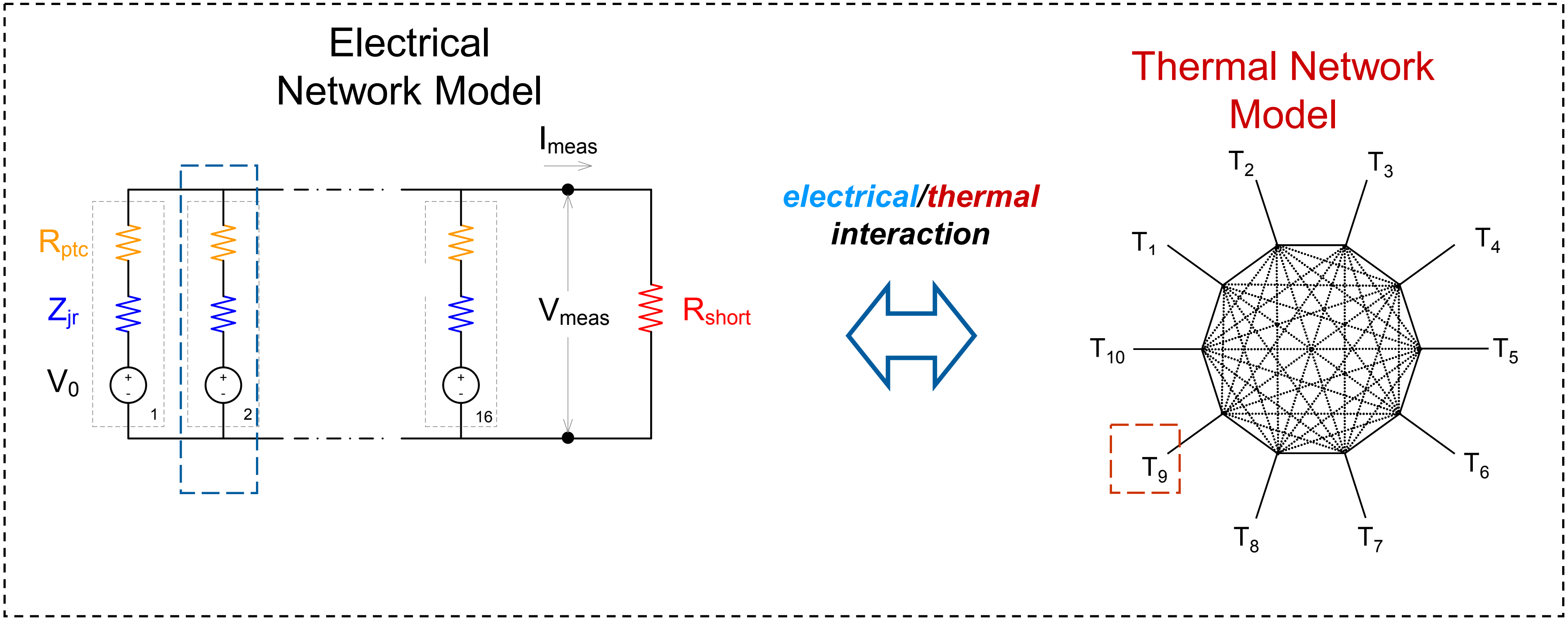
Unsteady Form

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

Model Development Approach

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

Multicell Thermal and Electrical Network Model

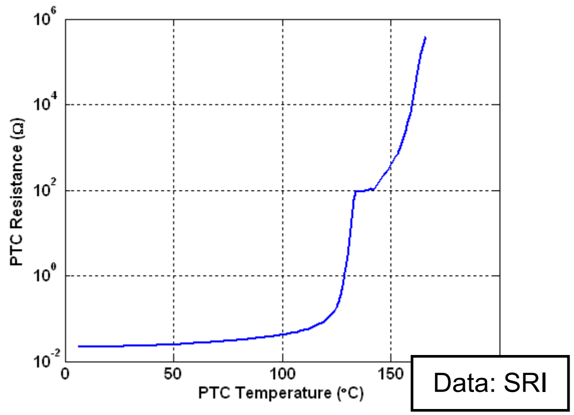


Multicell Network Model

Electrical Network Model

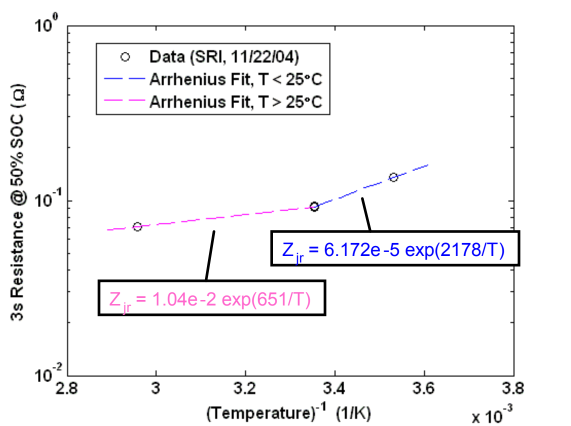
PTC Resistance

as a function of PTC temperature

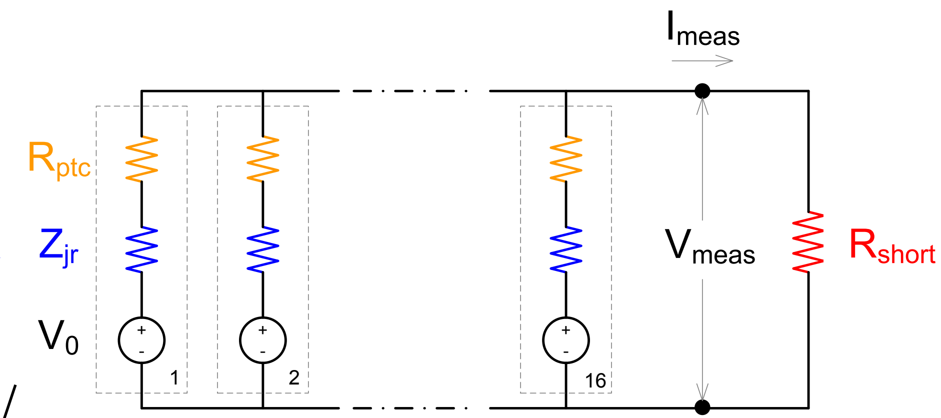


Jellyroll Resistance

as a function of cell temperature

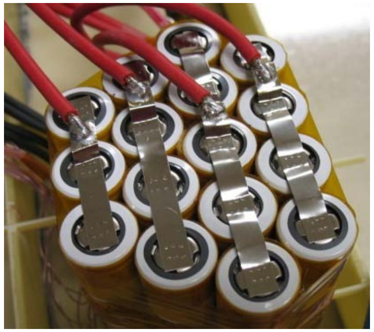


The model solves voltage and current interactions among the components in a multicell circuit.



Open-Circuit Voltage

as a function of cell SOC



Multicell 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

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

Staggered Array

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

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

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

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

$$F_n = 0$$

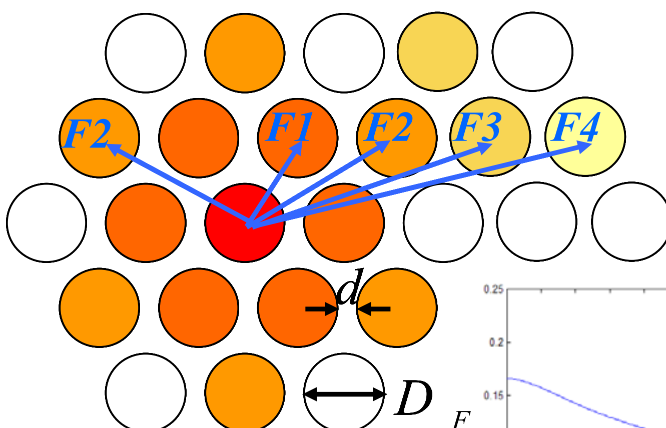
For $\frac{2}{\sqrt{3}} - 1 < \frac{d}{D} \le 1$, i.e. $\frac{2}{\sqrt{3}} < X \le 2$

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

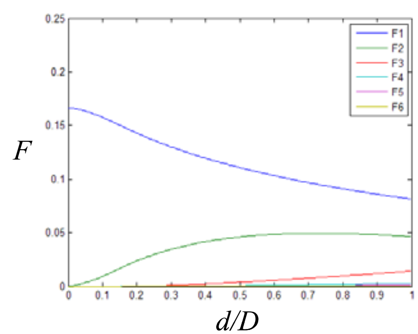
$$F_2 = \frac{1}{\pi}\left[\sqrt{3X^2-1} - 2\sqrt{X^2-1} + 2\cos^{-1}\left(\frac{1}{X}\right) - \cos^{-1}\left(\frac{1}{\sqrt{3}X}\right) - \frac{\pi}{6}\right]$$

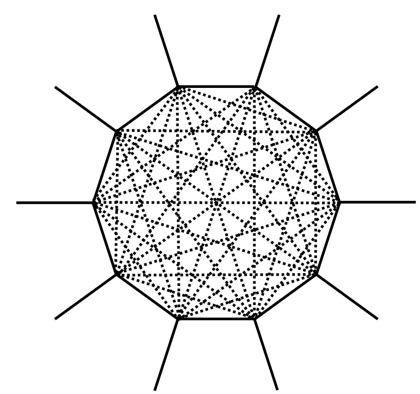
$$F_n = \frac{1}{2\pi}\left[\begin{array}{l}\sqrt{\{n(n-1)+1\}X^2-1} - 2\sqrt{\{(n-1)(n-2)+1\}X^2-1} + \sqrt{\{(n-2)(n-3)+1\}X^2-1} \\ -\cos^{-1}\left(\frac{1}{\sqrt{n(n-1)+1}X}\right) + 2\cos^{-1}\left(\frac{1}{\sqrt{(n-1)(n-2)+1}X}\right) - \cos^{-1}\left(\frac{1}{\sqrt{(n-2)(n-3)+1}X}\right) \\ +\tan^{-1}\left\{\frac{2}{\sqrt{3}}\left(n-\frac{1}{2}\right)\rig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

Radiation Heat Transfer



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





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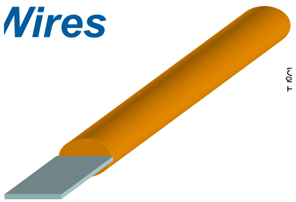
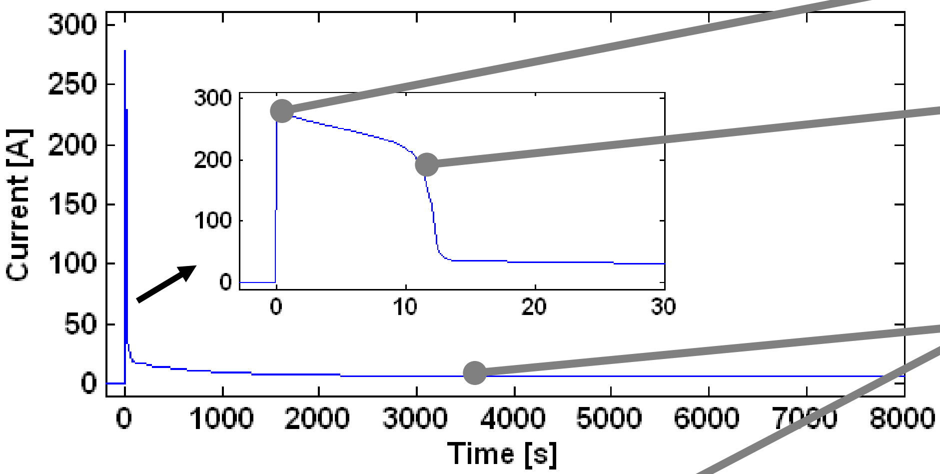
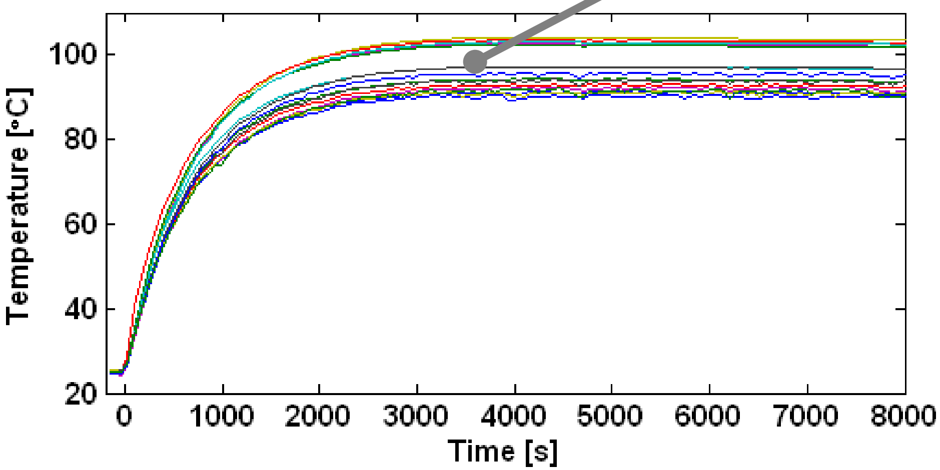


Experimental Model Validation

10 mΩ External Short

Data & Photo: SRI

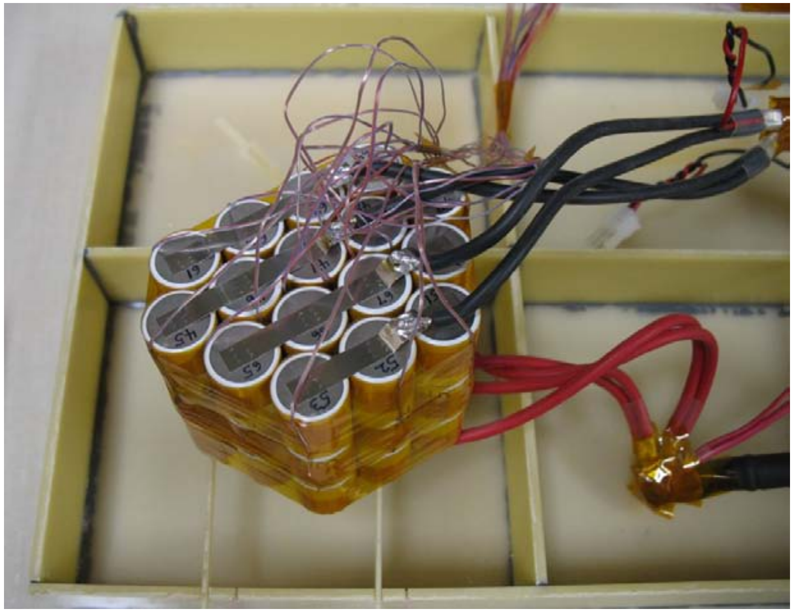




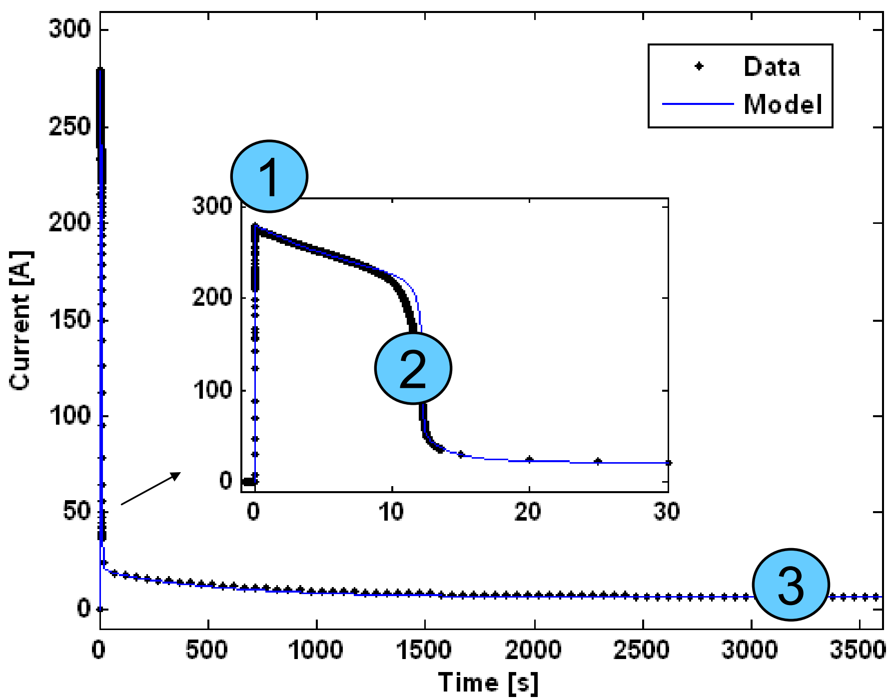
1) t = 0 sec: Circuit closed.

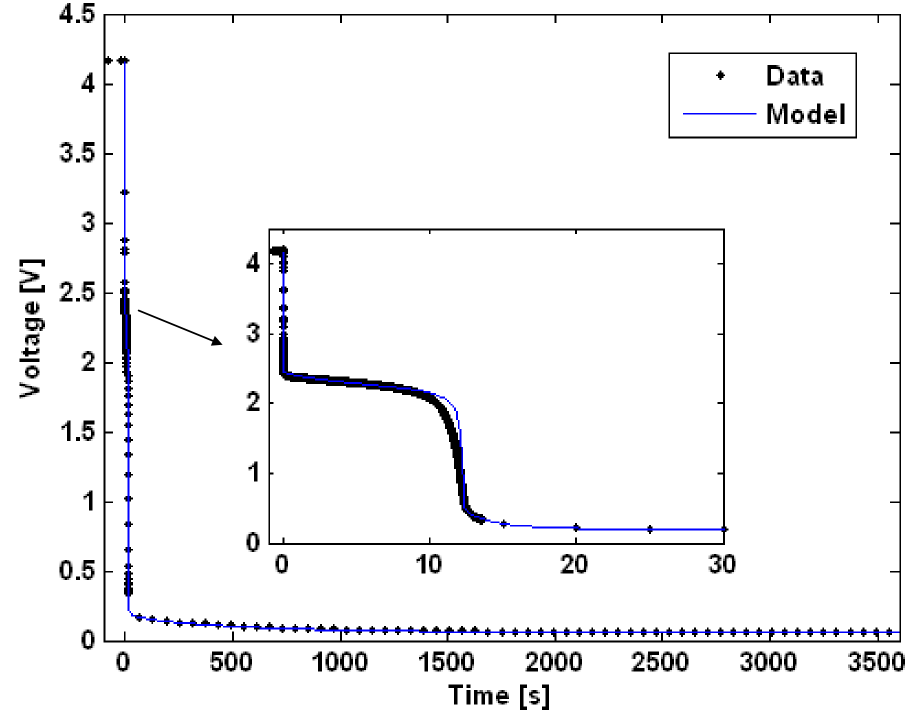
2) t ≈ 12 sec: PTC devices trip.
   - T_{PTC} = 130ºC

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



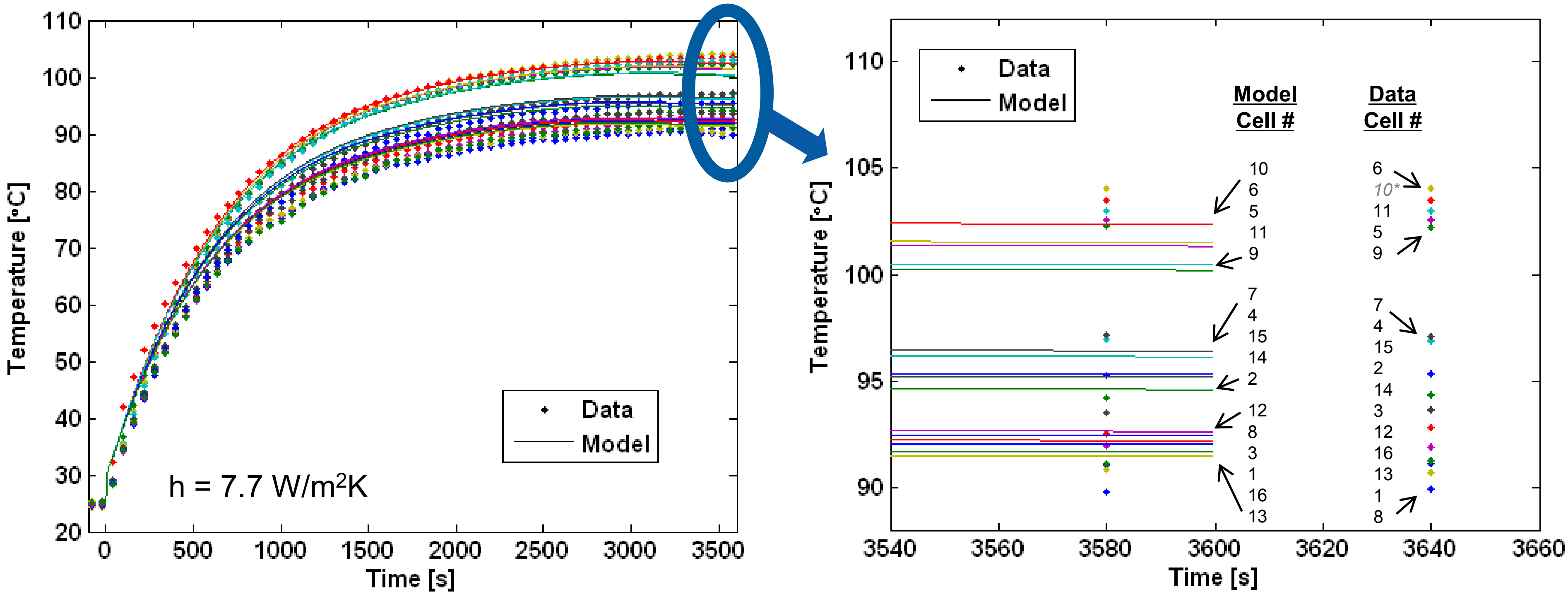
Model Validation – Current & Voltage

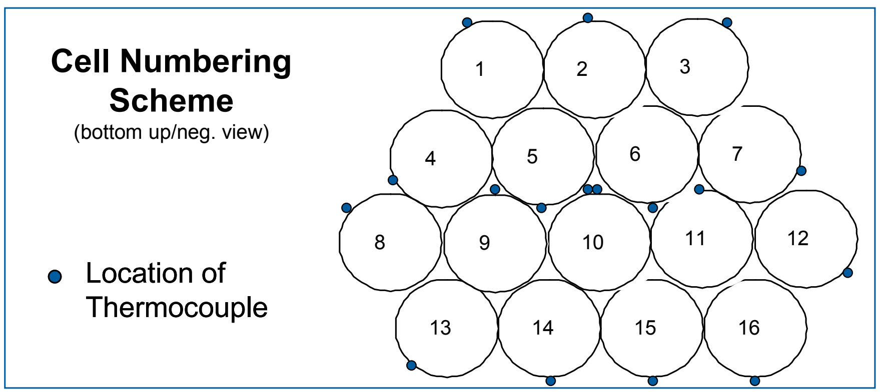




1. Peak inrush current readily predicted with knowledge of cell & short resistances.
2. PTC device trip time affected by
   - PTC thermal mass
   - PTC conductive path to jellyroll & can.
3. Steady-state behavior affected by jellyroll and PTC device temperature, indirectly:
   - PTC conductive path to jellyroll & can
   - Thermal boundary conditions to ambient.

Model Validation – Temperature



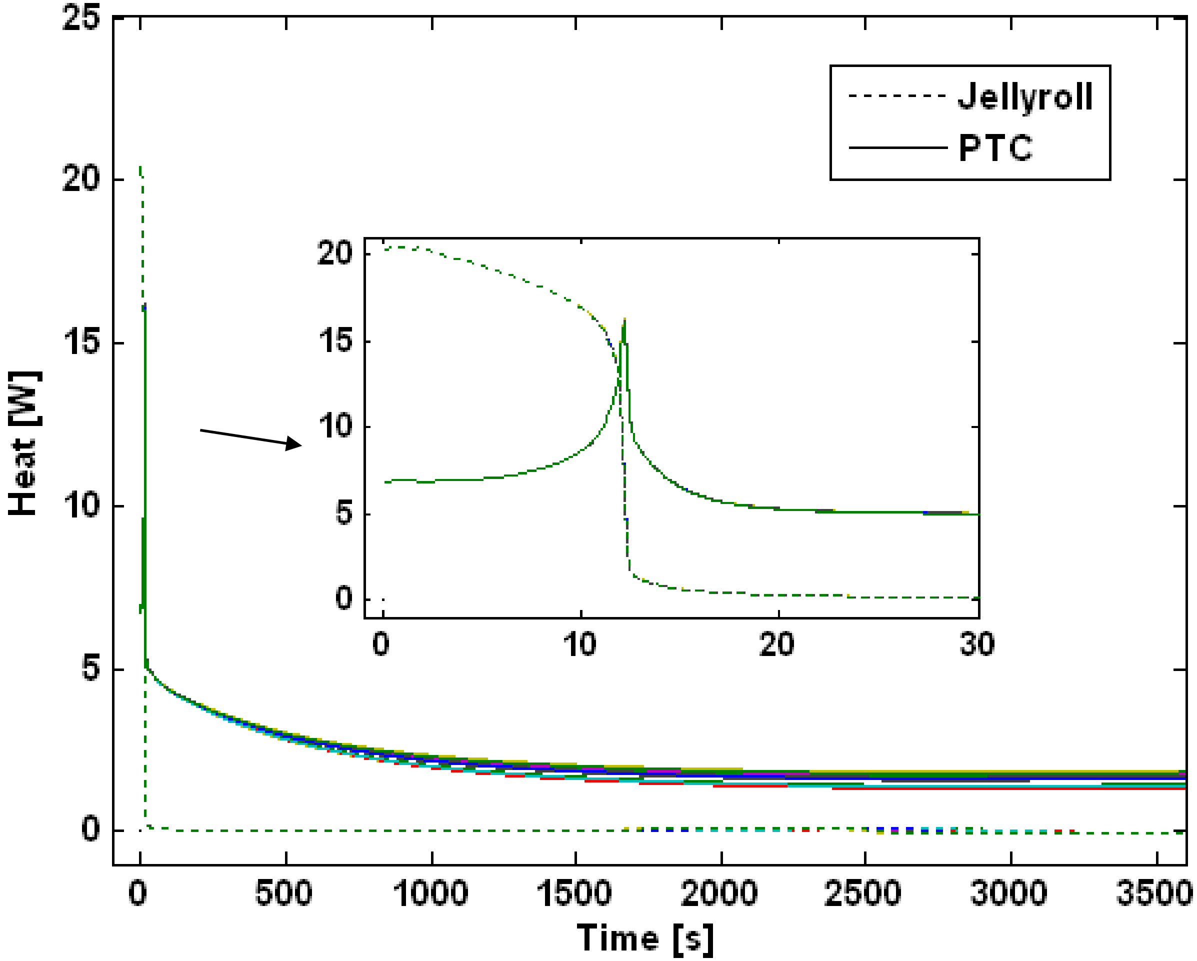


Model predicts correct temperature rise, but slightly smaller cell-to-cell ΔT caused by

- Model uniform T in cell-radial direction
- Thermocouple locations

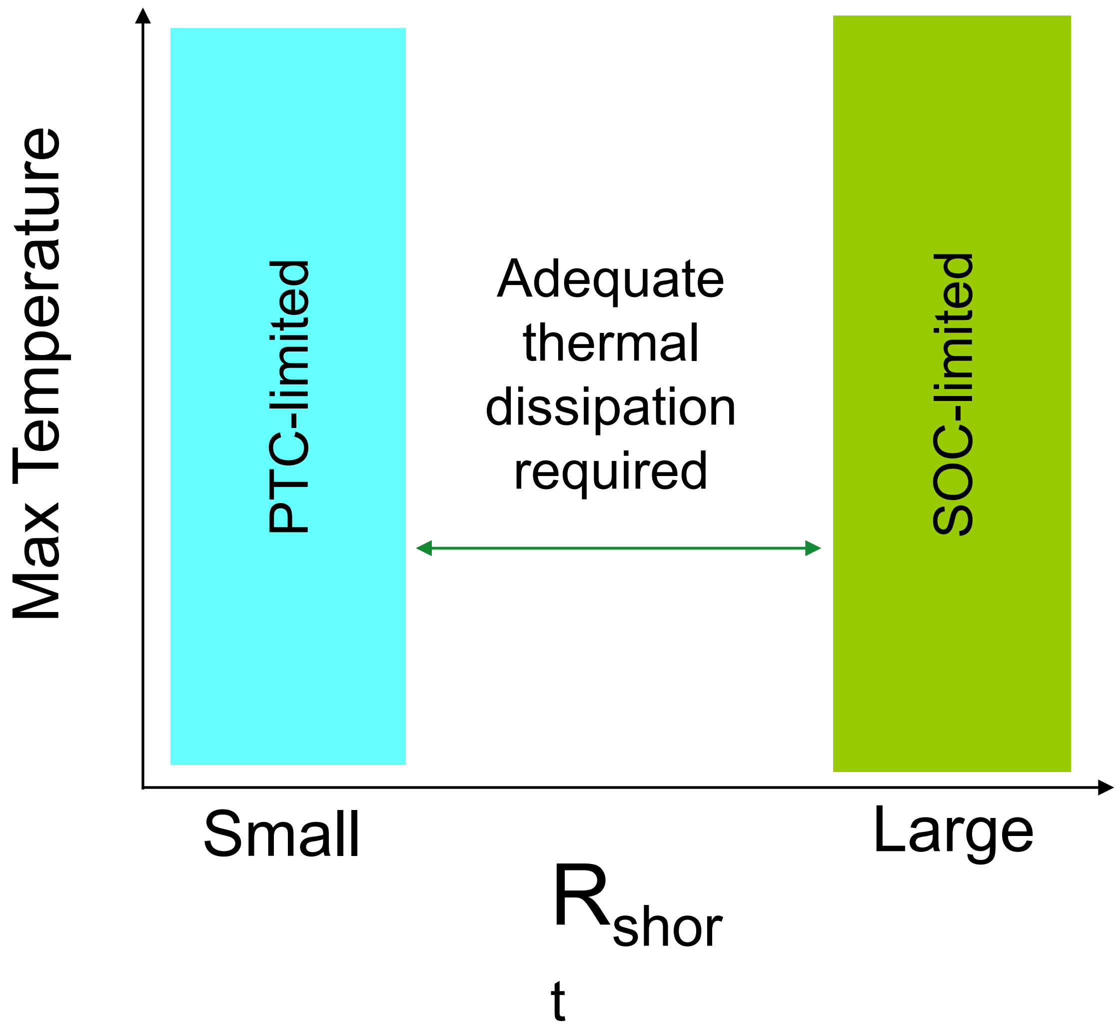
Model Prediction – Heat Generation

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

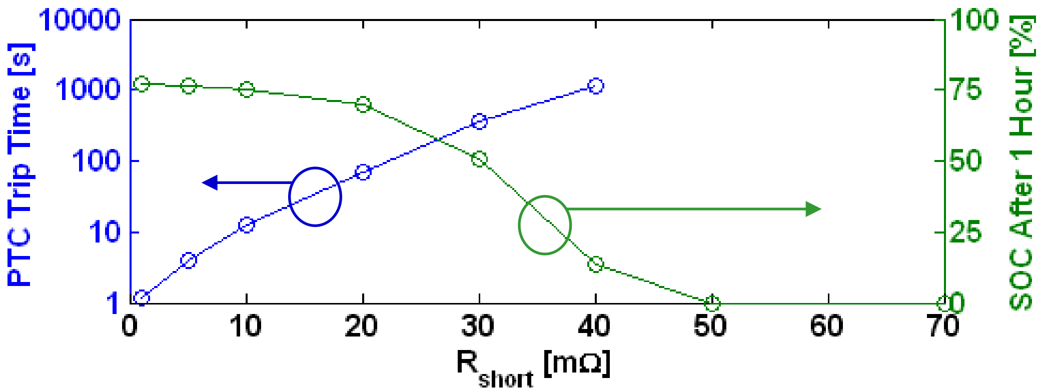


PTC devices at steady state 1.35 to 1.86 W

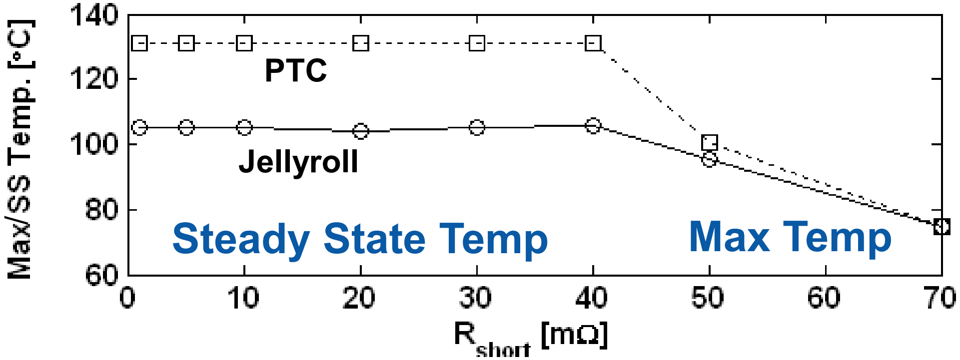
Is this design safe under other short conditions?



Simulation Results at Various Values of R_{short}



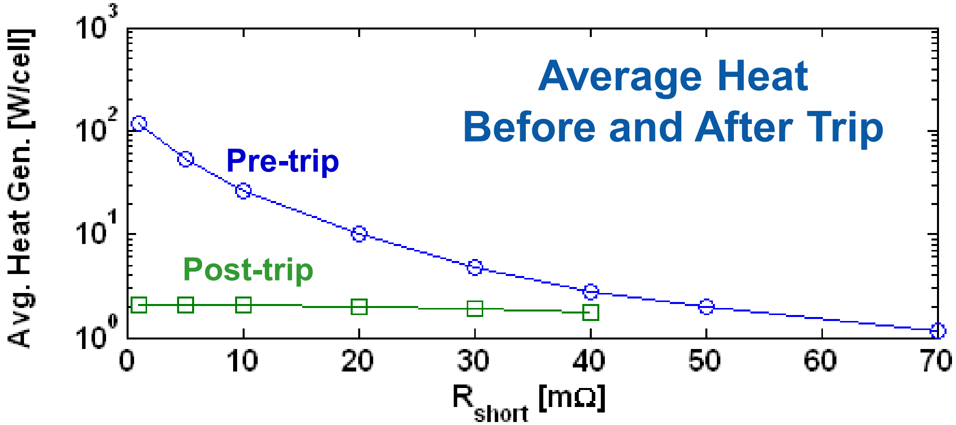
- $R_{short} \leq 40$ mΩ: PTC-limited
- $R_{short} \geq 50$ mΩ: SOC-limited



- 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)

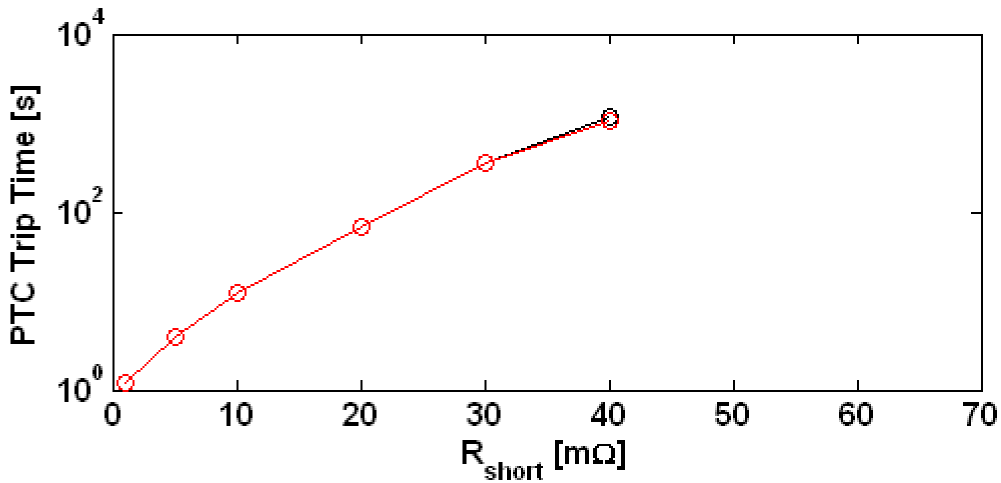


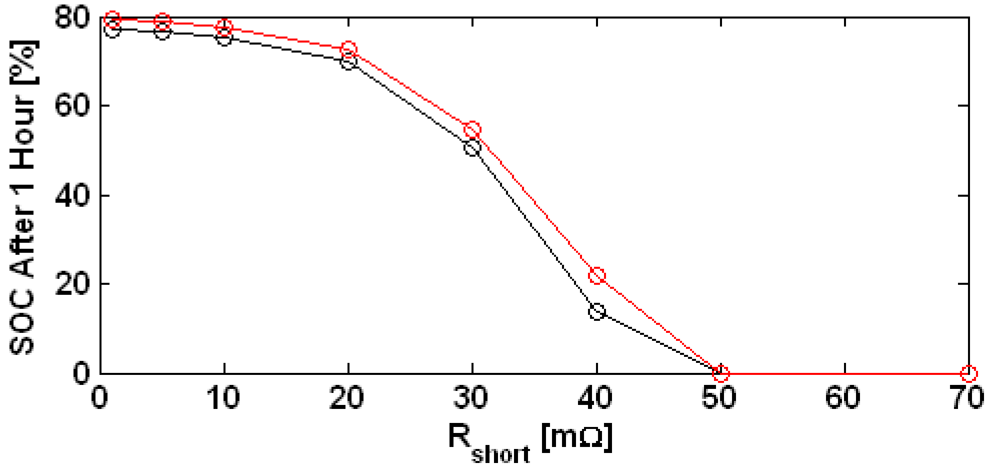
- Large pre-trip heat rates are safe provided that they have
  - Short duration
  - Sufficient thermal mass
  - Sufficient heat dissipation

How much heat rejection is required for safety?

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

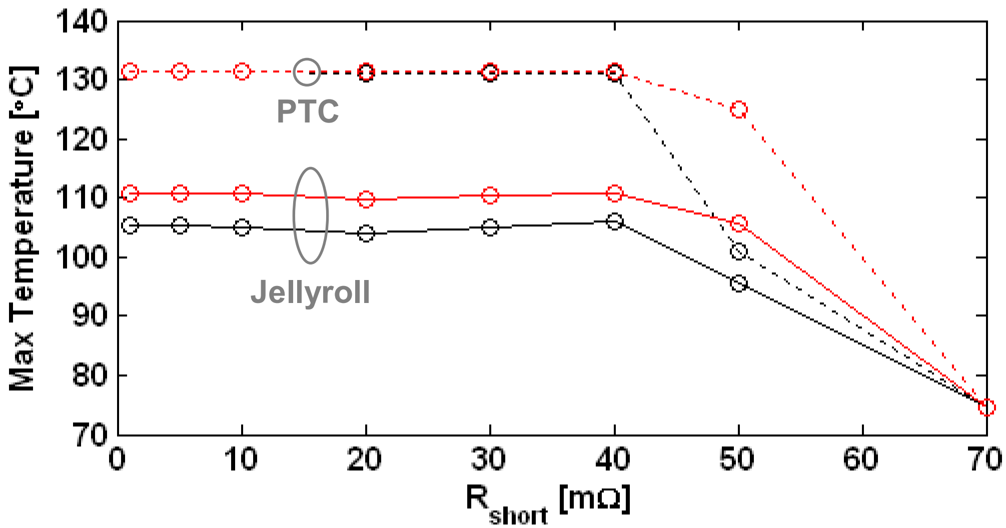
Red lines: $h = h_{nominal} / 2$
Black lines: $h = h_{nominal}$





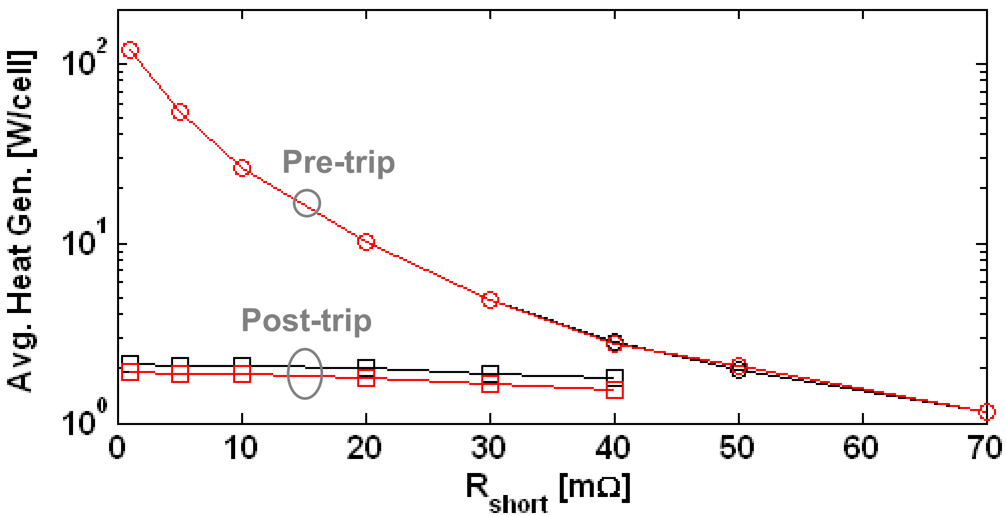
- PTC device trip time decreases only slightly with less heat rejection from cells.
- Less rejection leads to hotter PTC device (higher resistance) and slower discharge of cell.

How much heat rejection is required for safety?



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

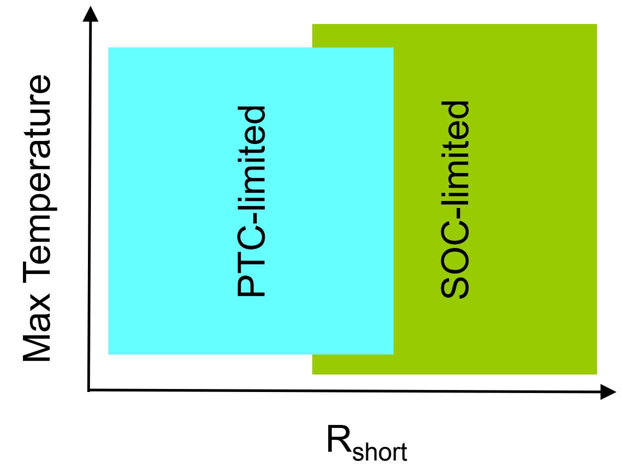
Black lines: h = $h_{nominal}$



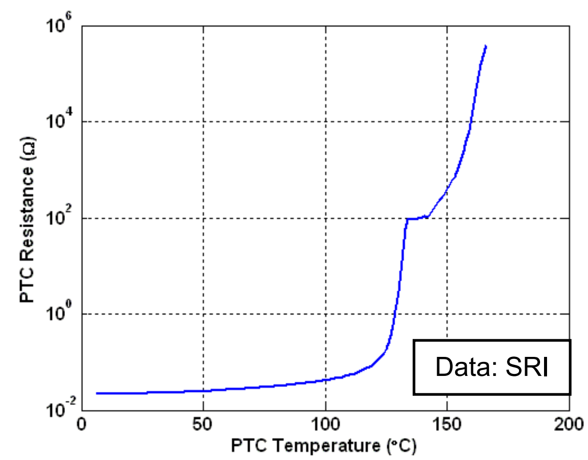
- Less rejection causes an increase in jellyroll temperature.
- Pre-trip heat generation rate largely unaffected by thermal boundary conditions.
- Post-trip, the PTC device reduces heat generation rate as heat rejection decreases.

Conclusions

- Created & validated a new multicell math model capturing electrical and thermal interactions of cells with PTC devices during abuse. Suitable for
  - Assessment of battery safety design margins
  - Supplement and guide verification tests



- Moli ICR18650J cell design has promise to be tolerant to a wide range of external shorts for the 16p configuration of spacesuit battery as long as
  - No damage due to the in-rush current transient occurs
  - Nominal tripping of cell PTC devices and steady state conditions occur



- 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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