



# SHORT COURSE ON LITHIUM-ION BATTERIES:

*~FUNDAMENTAL CONCEPTS, HEATING MECHANISMS AND SIMULATION TECHNIQUES~*

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## **SHORT COURSE OVERVIEW**

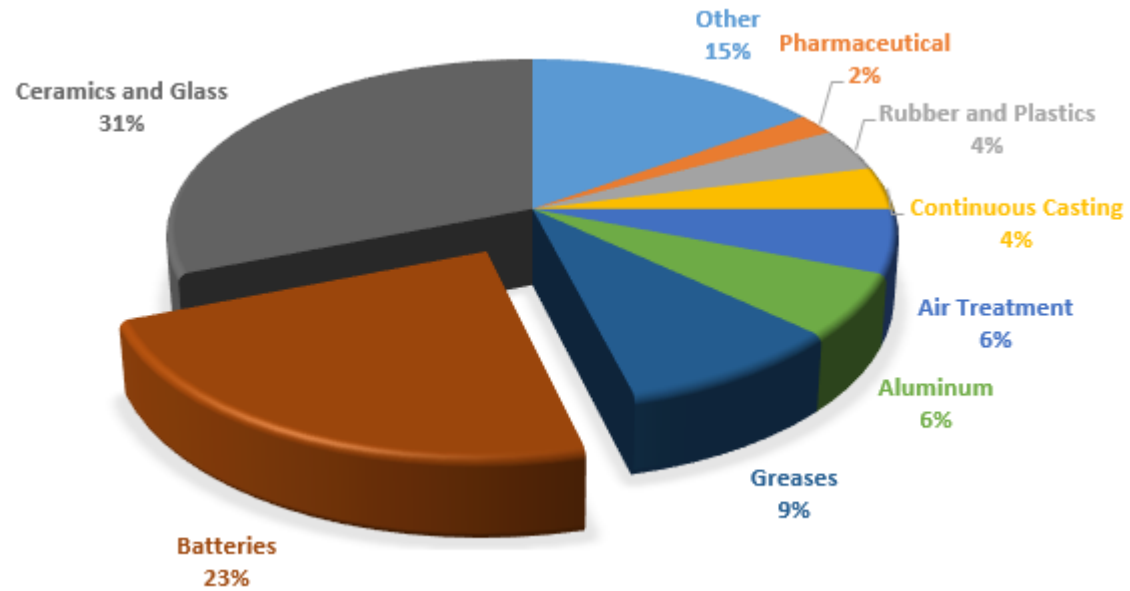
- **Section 1: Lithium-ion Battery Fundamentals**
- **Section 2: Heating Mechanisms Part 1: Ohmic Heating and Entropy**
- **Section 3: Heating Mechanisms Part 2: Thermal Runaway**

### **Break (10 minutes)**

- **Section 4: Simulation Techniques Part 1: Thermal Model Construction Methods**
- **Section 5: Simulation Techniques Part 2: Example Analysis Results**
- **Section 6: Acknowledgements**
- **Section 7: References**

# **SECTION 1: LITHIUM-ION BATTERY FUNDAMENTALS**

# LITHIUM-ION BATTERY FUNDAMENTALS: LITHIUM-ION BATTERIES ARE EVERYWHERE



Lithium battery end use breakdown based on data from Roskill Information Services LTD. 2009 estimates [1]



## LITHIUM-ION BATTERY FUNDAMENTALS: BATTERIES AND SPACE EXPLORATION

- **Lithium ion (Li-ion) batteries provide energy dense and low mass advanced energy storage solutions for a wide array of applications which include medical, industrial, railway, automobile, military and aerospace:**
  - Growing demand for advanced energy storage (AES) systems drives the Li-ion battery market which is expected to reach \$43 billion USD by 2020 [1, 5-7]
- **Space exploration applications depend on on safe and reliable AES and power management systems:**
  - Mission longevity depends on lightweight, safe, reliable and efficient AES
  - Energy in space is limited to finite quantities of resources:
  - Fuel is limited by storage tank size and launch mass limits
  - Cost per pound to orbit ranges between \$10k to \$55k [8]
- **Traditional alkaline based nickel cadmium (NiCd), nickel-metal hydride (NiMH) and nickel hydrogen (NiH<sub>2</sub>) batteries face replacement with Li-ion systems:**
  - Li-ion batteries offer more the double the performance for half the mass of their alkaline counterparts; Li is the lightest metal with an atomic mass of 6.94 amu
  - The International Space Station (ISS) begins replacing NiH<sub>2</sub> batteries with Li-ion batteries in November 2016
- **The number of international partners and new private companies in the space industry are growing:**
  - Space industry growth equates to increased usage and development of advanced Li-ion batteries

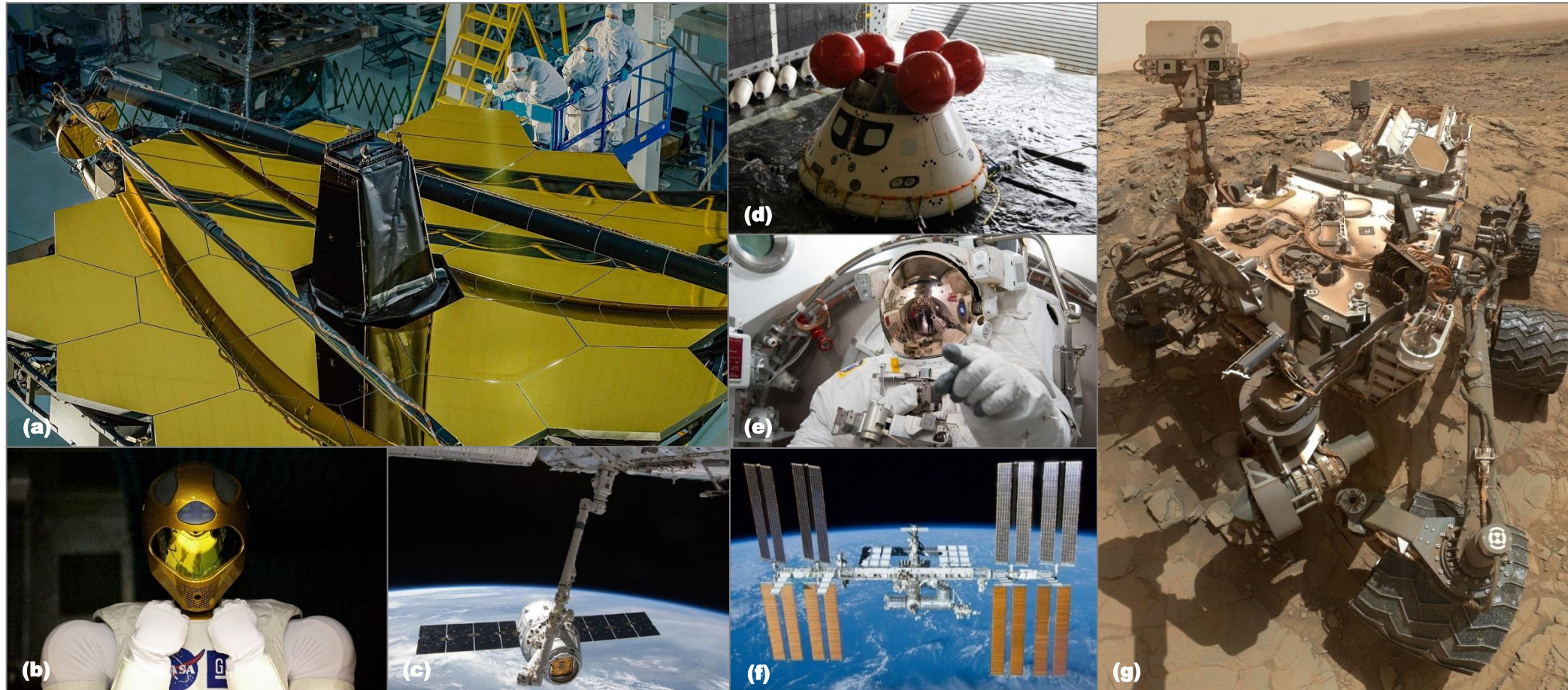


Images retrieved online from company websites. Examples of various industrial grade Li-ion battery manufacturers. This list is not comprehensive and does not indicate any opinion or preference of the presenter or their affiliation [9-22]



Images retrieved online from company websites. Examples of national agencies and various private industry competitors involved in space exploration. This list is not comprehensive and does not indicate any opinion or preference of the presenter or his affiliation [23-35].

# LITHIUM-ION BATTERY FUNDAMENTALS: BATTERIES AND SPACE EXPLORATION



Public domain images of space applications utilizing Li-ion technology: (a) James Webb Space Telescope, (b) Robonaut 2, (c) SpaceX Dragon, (d) Orion MPCV, (e) Extra-vehicular Mobility Unit, (f) ISS and (g) Mars Rover Curiosity. Credit for all images is attributed to NASA, except for image (e) where credit is given to the US Navy.

## LITHIUM-ION BATTERY FUNDAMENTALS: RELATING THE ELECTROCHEMICAL REACTIONS, ENERGY AND POTENTIAL

### ➤ The primary components of Li-ion batteries are the anode, cathode, electrolyte and separator

- Li ions intercalate/de-intercalate between the anode and cathode (i.e. electrodes) during discharge/charge respectively; intercalation refers to the insertion and extraction of ions between the layers of cathode/anode materials
- Ions flow through an ionically-conductive and electrically insulative separator to prevent shorting
- Electrons flow through an external circuit

### ➤ Li-ion batteries function with electrochemical reactions:

- Chemical reaction caused by or accompanied by an electrical current
- Reduction-oxidation reactions occur at electrodes
- Primary batteries: non-reversible reactions
- Secondary batteries: reversible reactions (rechargeable)

### ➤ Half cell reactions (individual electrode reactions) used to calculate cell voltage via energy and potential relationships described through:

- Gibbs Free Energy,  $\Delta G = -nFE$
- Nernst Equation,  $E = E^0 - \frac{RT}{nF} \ln Q_R$

### ➤ Example of half cell reactions, overall reaction, energy calculation and potential calculation provided to the right:

- Cathode (+): Lithium Cobalt Oxide ( $\text{LiCoO}_2$ )
- Anode (-): Lithium graphite ( $\text{LiC}_6$ )
- Electrolyte: Lithium hexafluorophosphate ( $\text{LiPF}_6$ )

### ➤ Coulomb (C-Rate): charge/discharge rate based on total capacity. Example for a 1 Amp-hour battery to the right:



$$\text{Potential} = E^+ - E^- = 4 \text{ V}$$

$$\Delta G = -1 * 96500 \text{ C mol}^{-1} * 4 \text{ V (i.e. } 4 \text{ J C}^{-1}\text{)}$$

$$\Delta G = -386 \text{ kJ} = -107.2 \text{ Wh mol}^{-1} @ 0.17 \text{ kg mol}^{-1}$$

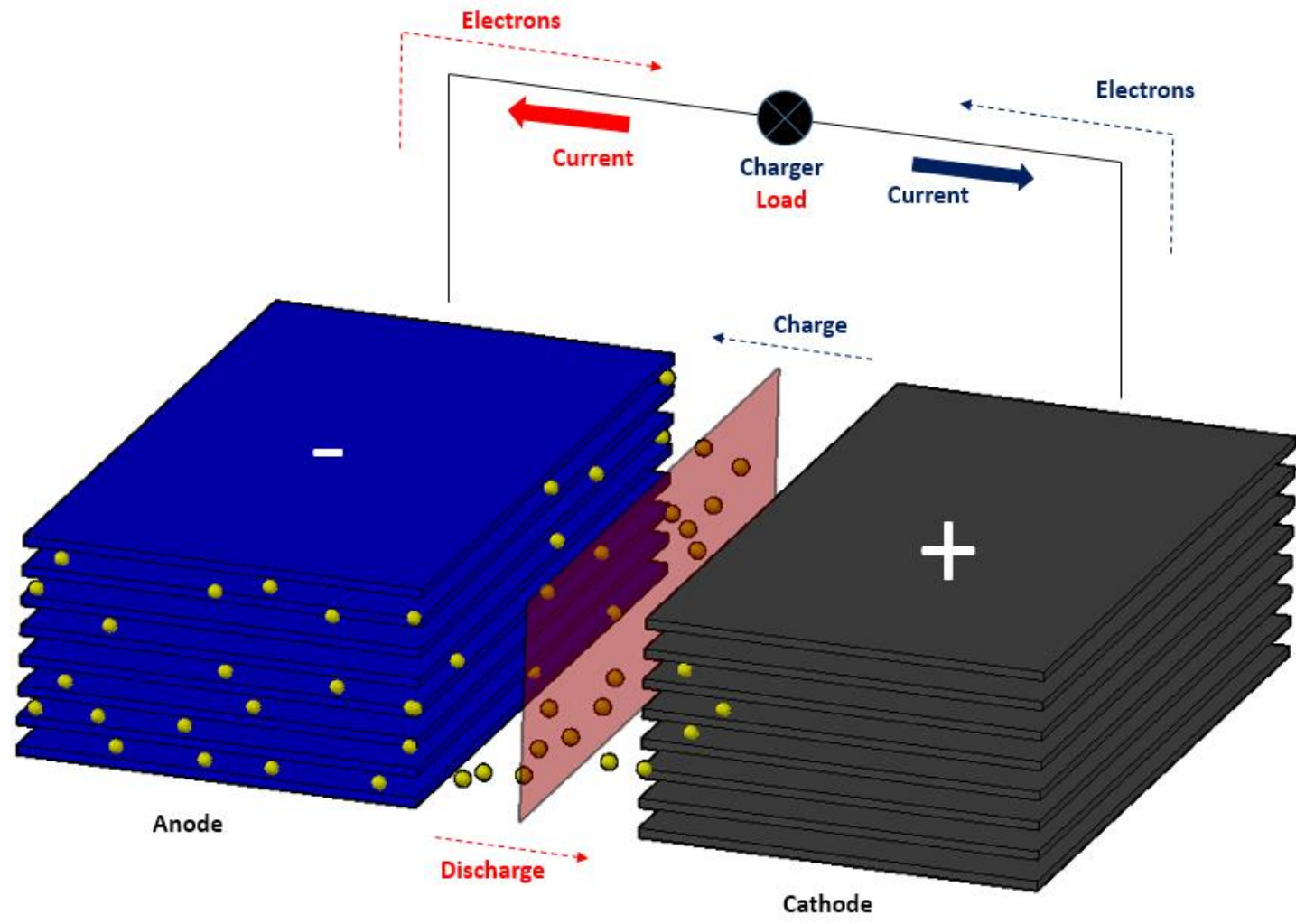
$$\text{Theoretical Specific Energy} = 630.6 \text{ Wh kg}^{-1}$$

$$2 \text{ C} = 2 \text{ A for 30 minutes (min)}$$

$$1 \text{ C} = 1 \text{ A for 1 hour (hr)}$$

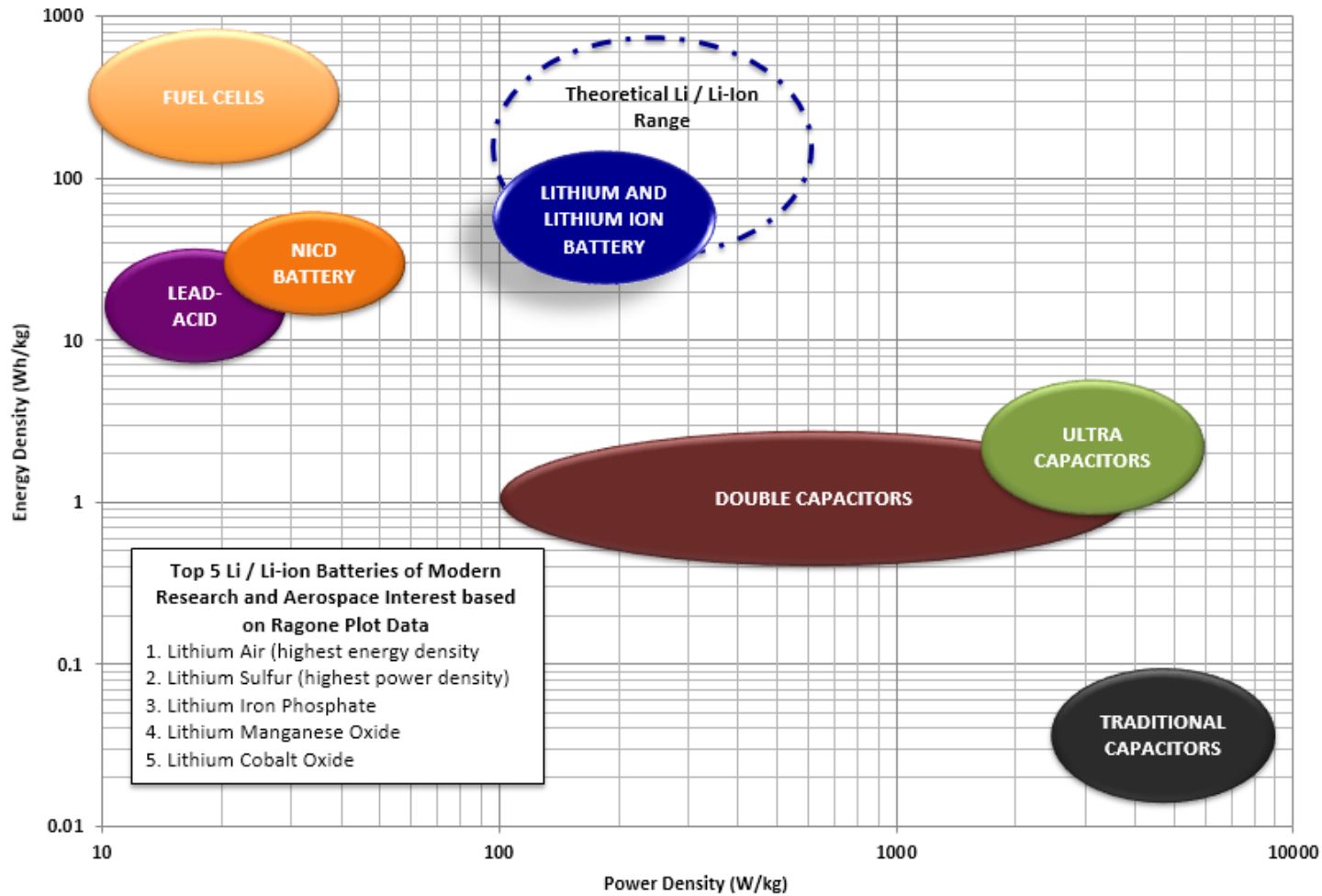
$$\text{C}/2 = 0.5 \text{ A for 2 hours (hrs)}$$

# LITHIUM-ION BATTERY FUNDAMENTALS: SCHEMATIC OF ION AND ELECTRON MOVEMENT





# LITHIUM-ION BATTERY FUNDAMENTALS: RAGONE PLOT



Ragone plot of energy storage device specific energy density vs. specific power density. Data adapted from the United States Defense Logistics Agency [36]

## **LITHIUM-ION BATTERY FUNDAMENTALS: DISADVANTAGES**

- **Cycling behavior and memory effect refer to the loss in capacity through cycling**
- **Poor cold temperature performance**
- **Solid Electrolyte Interphase (SEI) formation**
  - A passive layer consisting of organic and inorganic electrolyte decomposition products
  - Forms over anode surface during first charge cycle
  - Ion conducting, electrically insulating
  - Effects safety, cyclability, rate capability and induces irreversible charge loss
- **Volumetric expansion**
  - Too much volumetric change during insertion and de-insertion of Li ions can damage electrodes and detrimentally affect battery life and performance [43-44]
- **Other disadvantages center around safety concerns:**
  - Thermal runaway, which can occur due to mechanical failure, electrochemical failure or thermal failure (detailed discussion later)
  - Single cell thermal runaway energy can propagate to surrounding Li-ion cells causing a chain-reaction event
  - Ejected materials and gases during runaway events are toxic, acidic and highly dangerous (e.g. toxic organic electrolytes)



# **SECTION 2: HEATING MECHANISMS PART 1: OHMIC HEATING AND ENTROPY**

## HEATING MECHANISMS PART 1: OHMIC HEATING AND ENTROPY

- **Li-ion batteries generate heat during charge and discharge operations due to [45]:**
  - Differences in open circuit and working voltages
  - Changes in enthalpy terms and heat capacity
- **Bernardi et. al. (1985) [45] developed an energy balance to represent the local heat generated in a Li-ion cell:**
  - Voltage and current
  - Enthalpy of reaction (enthalpy voltage of reaction)
  - Enthalpy of mixing
  - Phase change
  - Heat capacity change
- **Bernardi's energy balance is commonly simplified to only include Ohmic losses (primary thermal driver):**

### A General Energy Balance for Battery Systems [45]

D. Bernardi,\*\* E. Pawlikowski,\* and J. Newman\*

*Department of Chemical Engineering, University of California, Berkeley, California 94720*

#### ABSTRACT

A general energy balance for battery systems has been developed. This equation is useful for estimating cell thermal characteristics. Reliable predictions of cell temperature and heat-generation rate are required for the design and thermal management of battery systems. The temperature of a cell changes as a result of electrochemical reactions, phase changes, mixing effects, and joule heating. The equation developed incorporates these effects in a complete and general manner. Simplifications and special cases are discussed. The results of applying the energy balance to a mathematical model of the LiAl/FeS cell discharged through two different reaction mechanisms are given as examples. The examples illustrate how the energy equation may be applied to a specific system to examine the relative contributions corresponding to the terms in the equation. The examples show that the processes involved in cell heat generation may be complex and that the application of a sufficiently general energy equation is advantageous.

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

## HEATING MECHANISMS PART 1: OHMIC HEATING AND ENTROPY (DISCHARGE EXAMPLE)

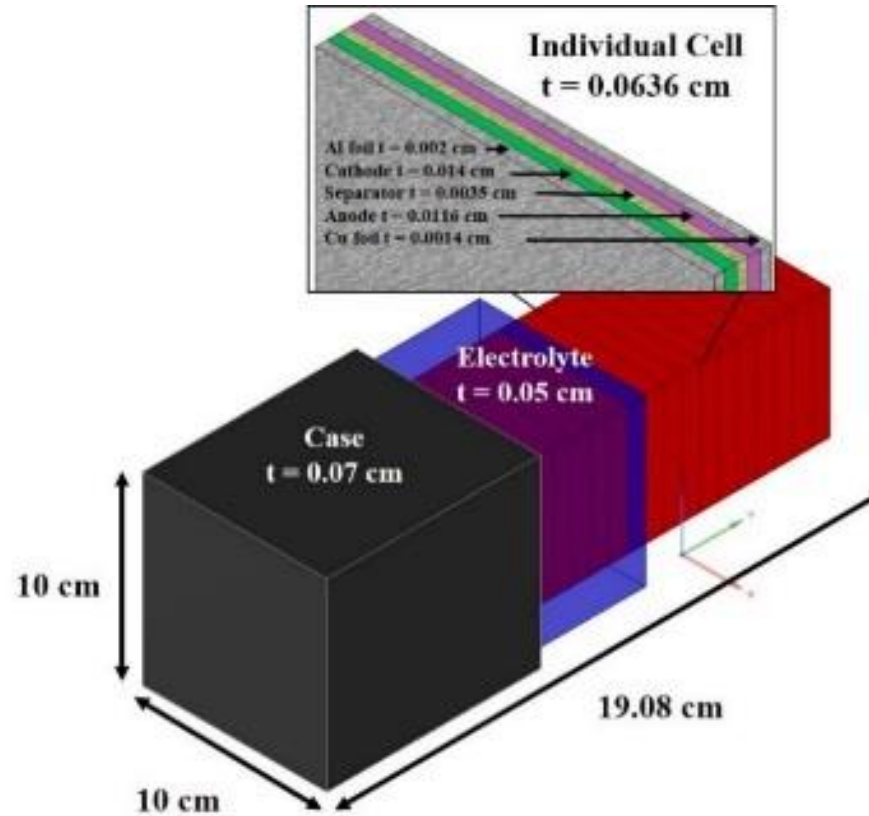
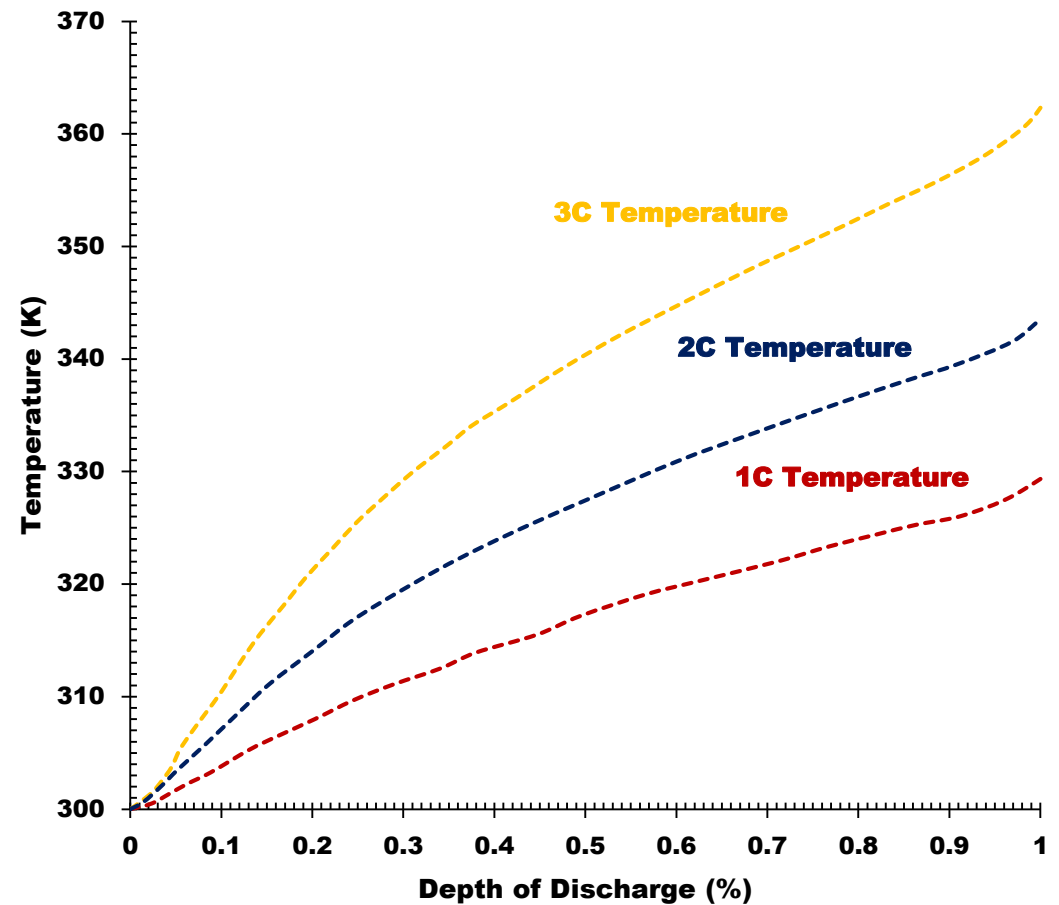
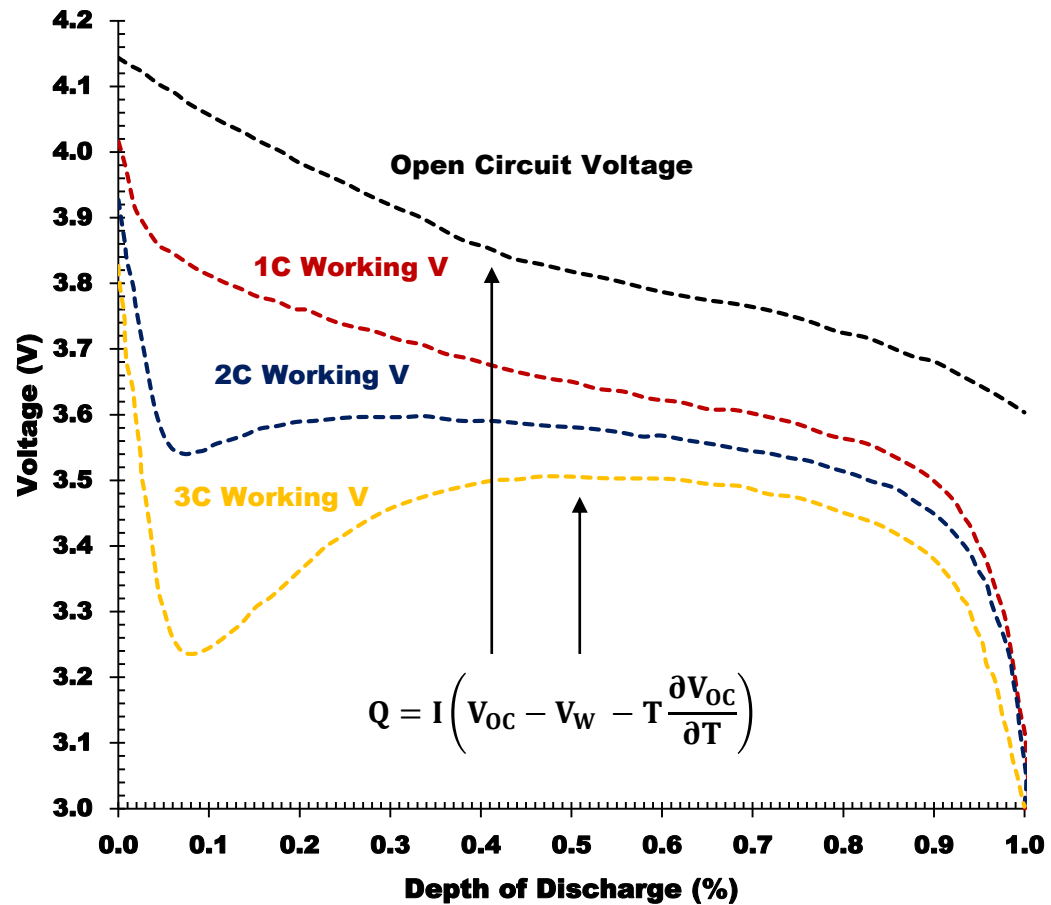


Image of a large format 185 Ah LiCoO<sub>2</sub> electric vehicle battery. Image adapted from Walker et. al. (JPS 2015) based on images by Chen et. al. (JPS 2005) [46-47].

# HEATING MECHANISMS PART 1: OHMIC HEATING AND ENTROPY (DISCHARGE EXAMPLE)



Voltage and temperature data from discharge of a large format 185 Ah LiCoO<sub>2</sub> electric vehicle battery. Plots adapted from Walker et. al. (JPS 2015) based on data by Chen et. al. (JPS 2005) [46-47].

# HEATING MECHANISMS PART 1: OHMIC HEATING AND ENTROPY (CHARGE EXAMPLE)

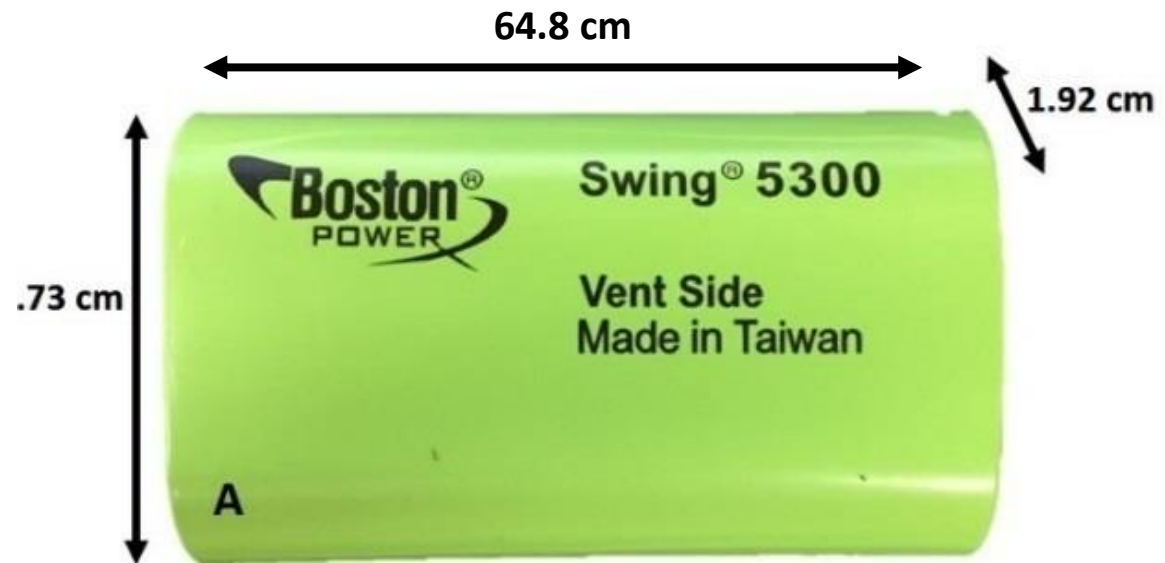
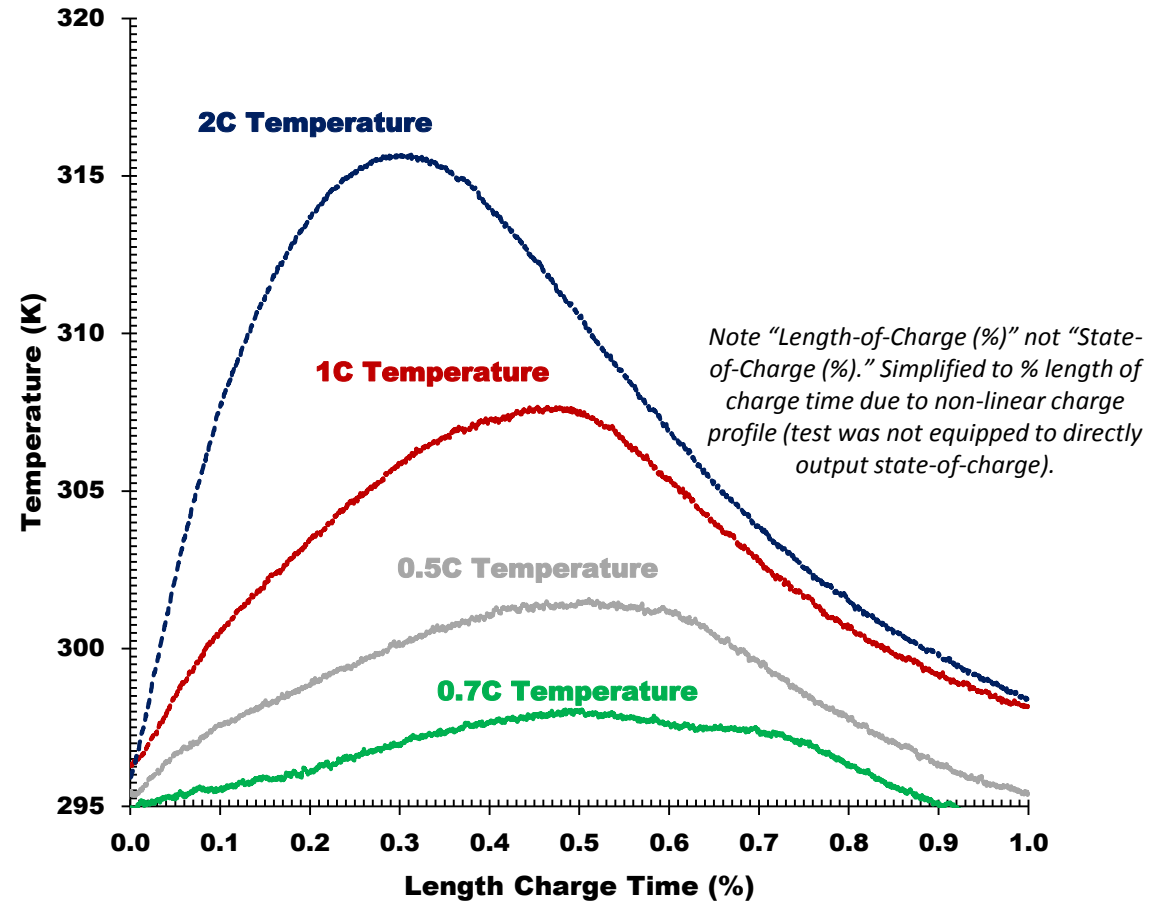
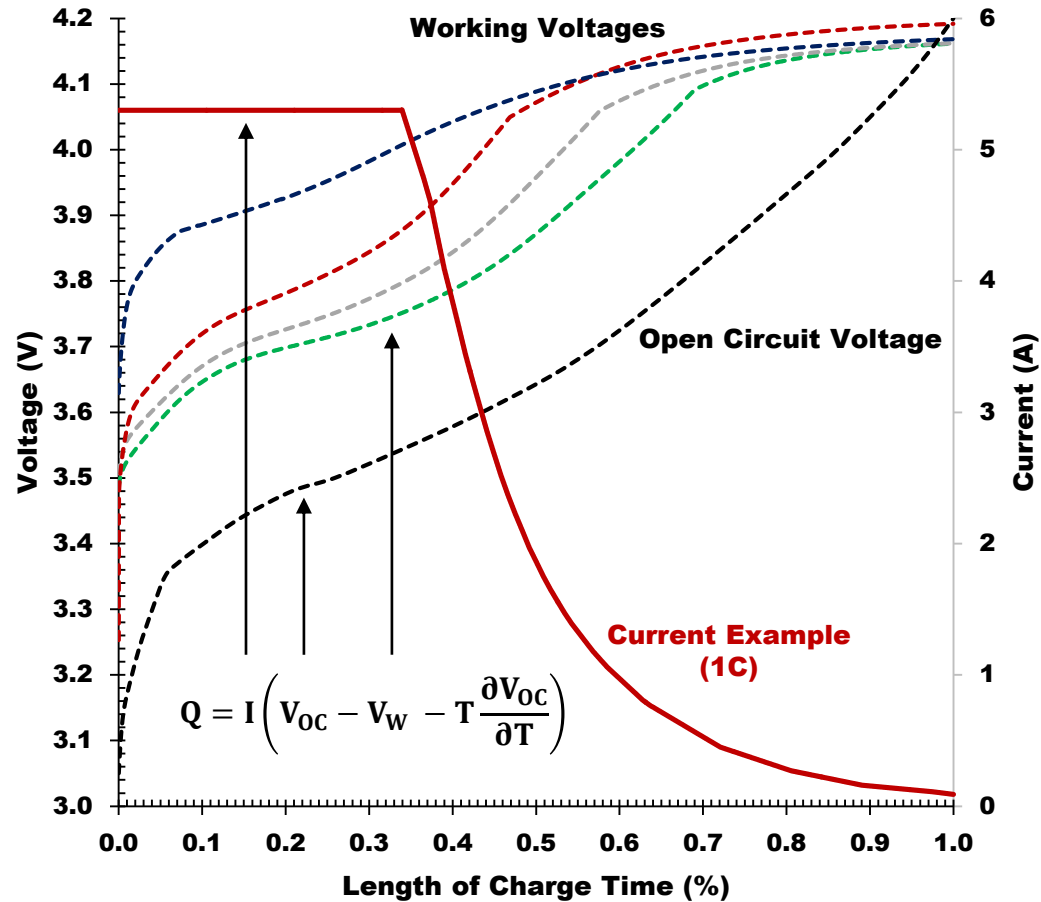


Image of a Boston Power Swing 5300 Li-ion cell [48-49].

# HEATING MECHANISMS PART 1: OHMIC HEATING AND ENTROPY (CHARGE EXAMPLE)



Voltage, current and temperature data from discharge of a 5300 mAh Boston Power Swing 5300 Li-ion battery. Data adapted from Walker et. al. (JPS 2015) [48-49].

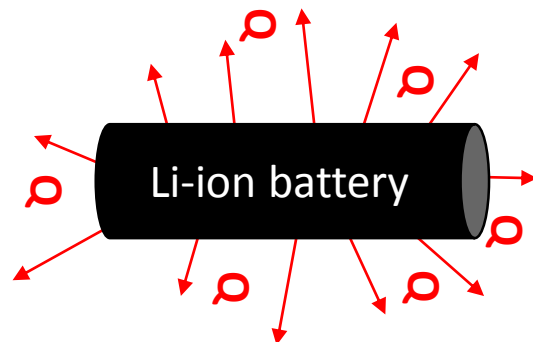




# SECTION 3: HEATING MECHANISMS PART 2: THERMAL RUNAWAY

# HEATING MECHANISMS PART 2: THERMAL RUNAWAY

- **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)
  - Electrochemical failure (e.g. internal shorting)
  - Electrochemical abuse (e.g. overcharge)
- **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 reactions heating rates are provided to the right:
- **Propagation is a chain reaction event which occurs when neighbor cells go into thermal runaway due to the energy released from the original runaway due event**



### Richard and Dahn (1999)

$$\frac{dx_{SEI}}{dt} = -A_{SEI} x_{SEI} \exp\left(\frac{-E_{SEI}}{k_b T}\right) \quad (1)$$

$$\frac{dx_a}{dt} = -A_a x_a \exp\left(\frac{-z}{z_0}\right) \exp\left(\frac{-E_a}{k_b T}\right) \quad (2)$$

$$\frac{dz}{dt} = A_a x_a \exp\left(\frac{-z}{z_0}\right) \exp\left(\frac{-E_a}{k_b T}\right) \quad (3)$$

$$\frac{dQ_{SEI}}{dt} = -m_{SEI} h_{SEI} \frac{dx_{SEI}}{dt} \quad (4)$$

$$\frac{dQ_a}{dt} = -m_a h_a \frac{dx_a}{dt} \quad (5)$$

Heating due to SEI and anode decomposition

### Hatchard et. al. (2001)

$$\frac{dx_c}{dt} = A_c x_c (1 - x_c) \exp\left(\frac{-E_c}{k_b T}\right) \quad (6)$$

$$\frac{dQ_c}{dt} = m_c h_c \frac{dx_c}{dt} \quad (7)$$

Heating due to cathode decomposition

### Kim et. al. (2007)

$$\frac{dy_e}{dt} = -A_e y_e \exp\left(\frac{-E_e}{k_b T}\right) \quad (8)$$

$$\frac{dQ_e}{dt} = -m_e h_e \frac{dy_e}{dt} \quad (9)$$

Heating due to electrolyte decomposition

### Coman et. al. (2015)

$$\frac{dSoC}{dt} = -A_{ec} (1 - x_c) x_a \exp\left(\frac{-E_{ec}}{k_b T}\right) + \left(\frac{dx_c}{dt} - \frac{dx_a}{dt}\right) SoC \quad (10)$$

$$\frac{dQ_{ec}}{dt} = -(m_c + m_a) h_{ec} \frac{dSoC}{dt} \quad (11)$$

Heating due release of electrochemical energy

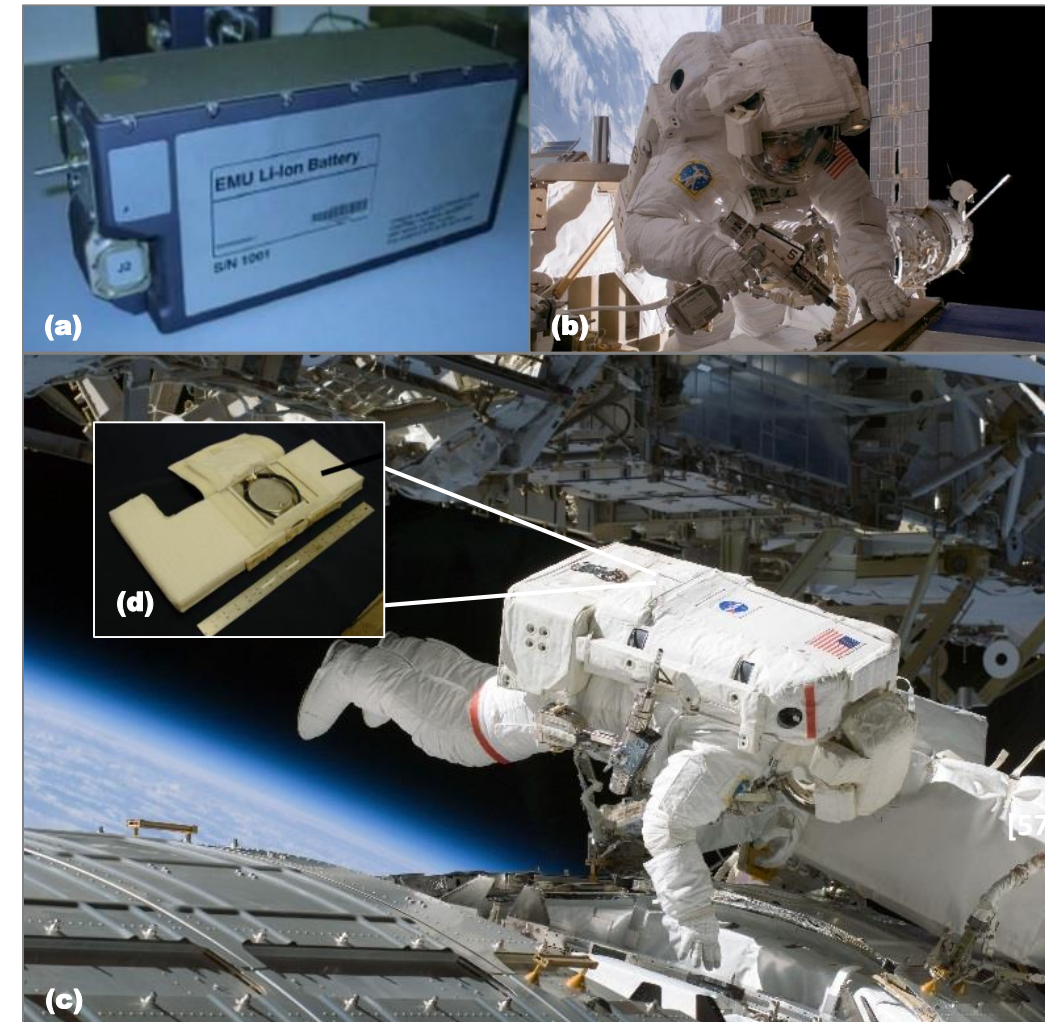
## HEATING MECHANISMS PART 2: THERMAL RUNAWAY ACCIDENTS



Online images of thermal runaway events for: (a) Hoverboard, (b) UPS Airlines Flight 6, (c) Tesla, (d) Boeing 787 Dreamliner image 1, (e) Boeing 787 Dreamliner image 2 and (f) Boeing 787 Dreamliner image 3.

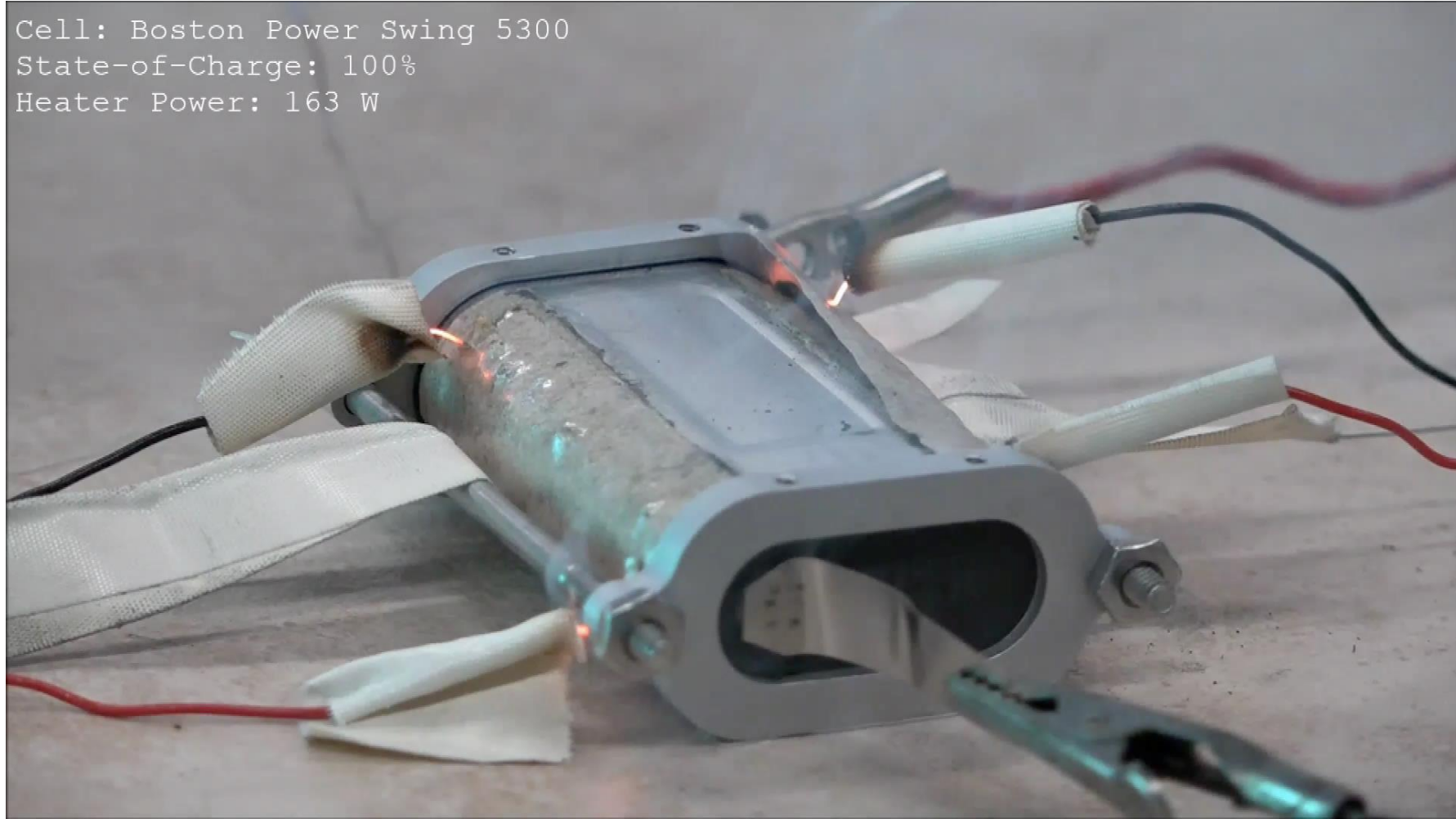
## HEATING MECHANISMS PART 2: NASA'S RESPONSE TO THERMAL RUNAWAY

- **Following the Boeing 787 Dreamliner incident, the NASA Engineering and Safety Center (NESC) was tasked to address safety concerns associated with Li-ion batteries and thermal runaway [58]:**
  - Li-ion Rechargeable Extravehicular Activity battery assembly (LREBA)
  - Li-ion Pistol Grip Tool battery assembly (LPGT)
  - Long Life Battery (LLB) for EMU
- **NASA NESC definition of design success:**
  - Assume thermal runaway will eventually happen
  - Design should ensure that TR event is not catastrophic
  - Demonstrate that propagation to surrounding cells will not occur
- **Thermal management systems designed to mitigate the effects of thermal runaway and prevent cell-to-cell propagation should consider the following [58]:**
  - No runaway event is the same; even for the same manufacturer and state-of-charge; there is a range of possible outcomes
  - Onset temperature, acceleration temperature, trigger temperature, trigger cell peak temperature and neighbor cell peak temperature
  - Total energy released through sides and top of the cell body
  - Cell failure type (e.g. side wall vs. top)
  - System pressure increase, gases released and ejecta material



Public access images representing the EMU Li-ion batteries evaluated by the NESC: (a) LLB, (b) LPGT, (c) EMU LREBA image 1, (d) EMU LREBA image 2 [58].

## HEATING MECHANISMS PART 2: THERMAL RUNAWAY EXAMPLE



## HEATING MECHANISMS PART 2: THERMAL RUNAWAY EXAMPLE

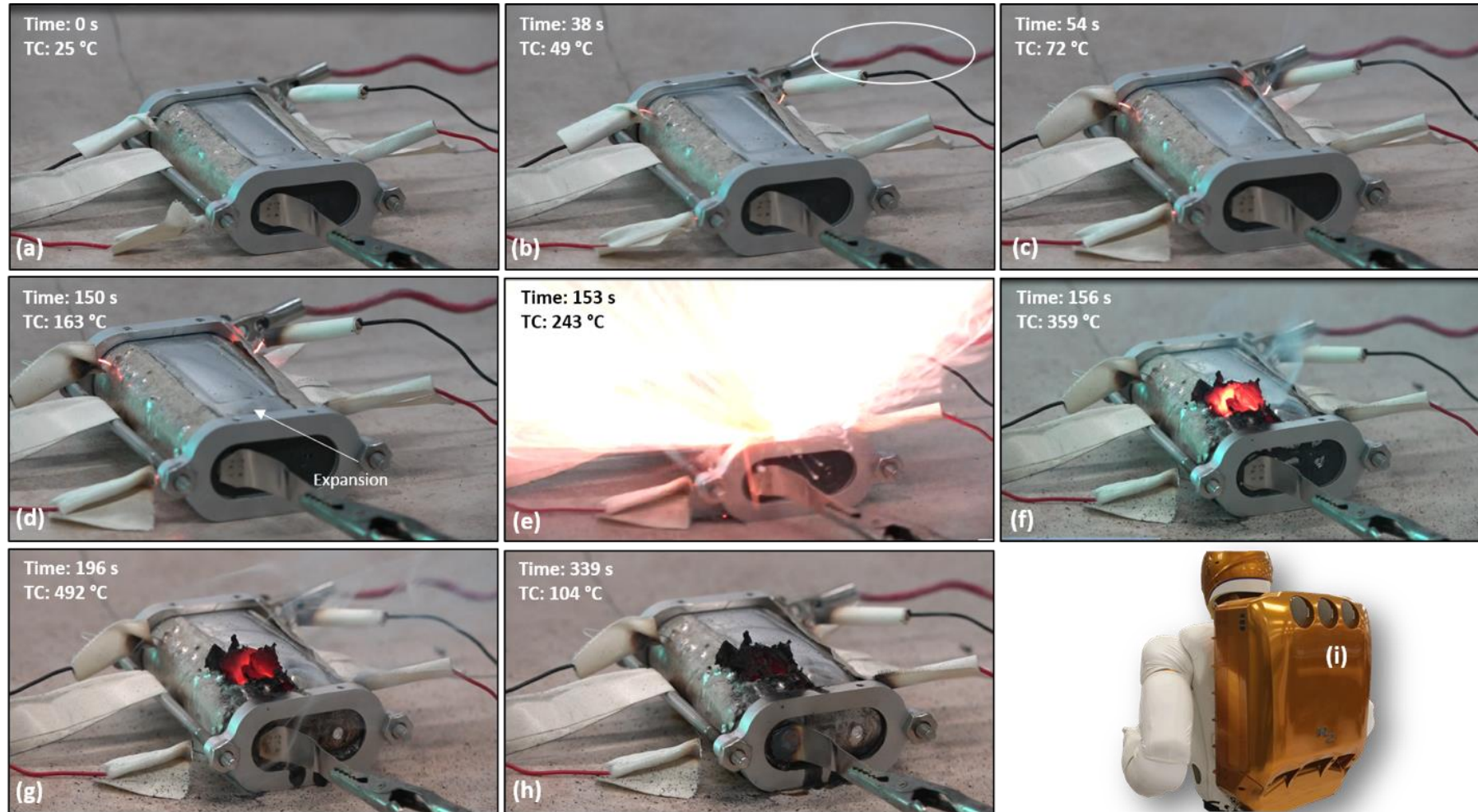
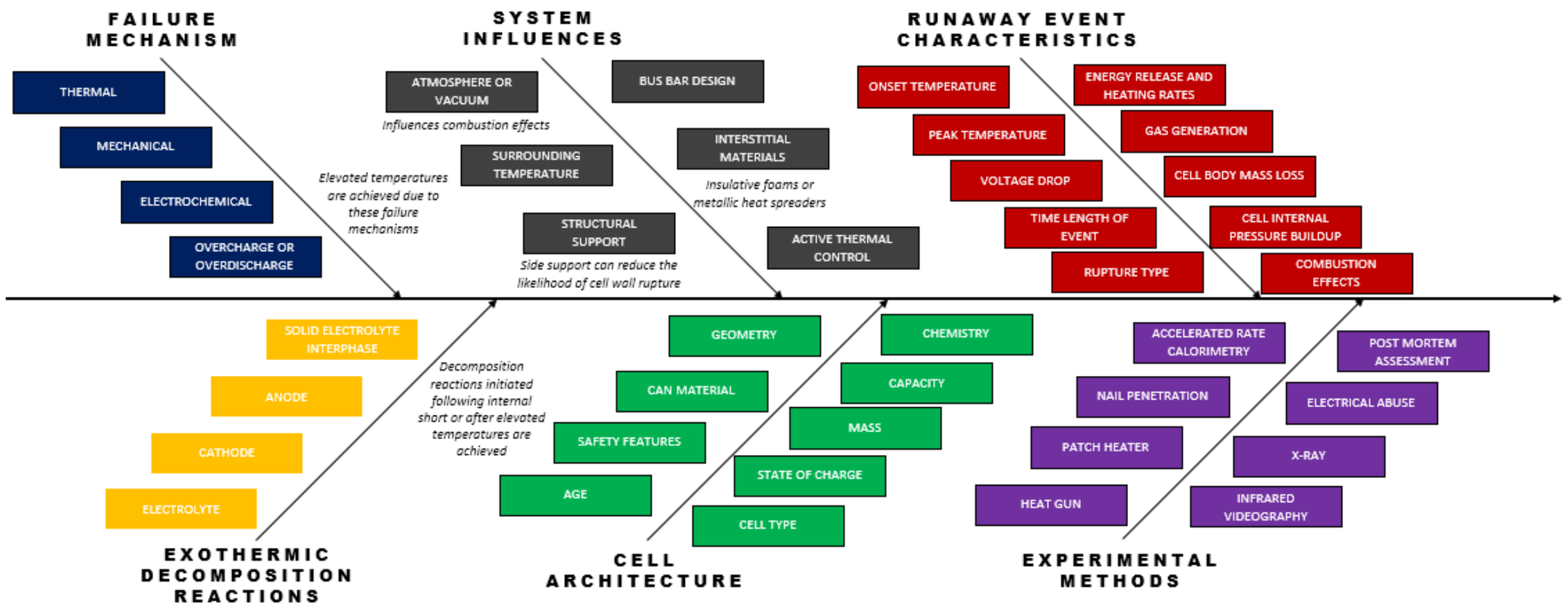


Image extracted from Sandeep et. al. "Energy Distributions Exhibited during Thermal Runaway of Commercial Lithium Ion Batteries used for Human Spaceflight Applications." Submitted to JPS April 2016 [59].

# HEATING MECHANISMS PART 2: UNDERSTANDING THERMAL RUNAWAY



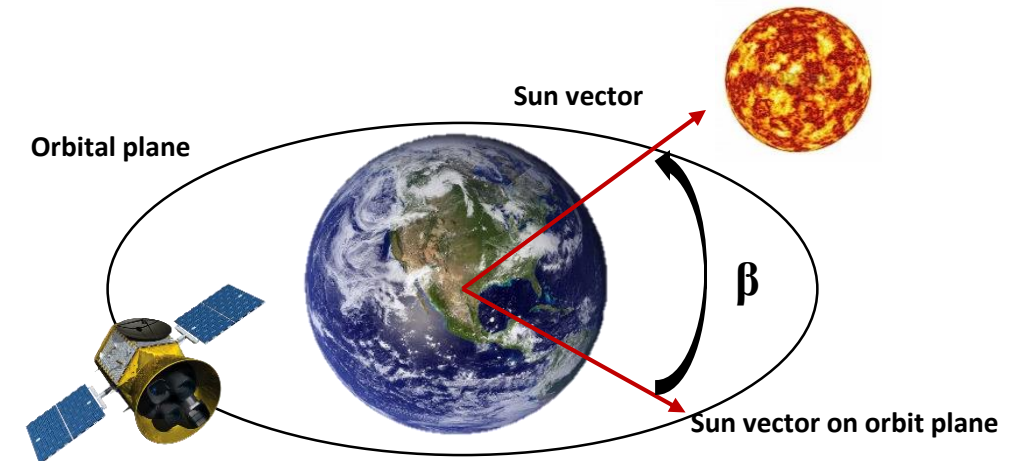
**BREAK TIME!**



# **SECTION 4: SIMULATION TECHNIQUES PART 1: THERMAL MODEL CONSTRUCTION METHODS**

## SIMULATION TECHNIQUES PART 1: THERMAL MODEL CONSTRUCTION METHODS

- **Li-ion battery performance, efficiency and safety are heavily influenced by cell temperature and surrounding temperature**
- **Understanding thermal performance via detailed thermal models can significantly help with the design process**
- **Accurate prediction of Li-ion battery thermal performance requires advanced test-correlated thermo-electrochemical models**
  - Generally, the optimal way to perform thermo-electrochemical analysis is with a multi-physics methodology, however;
  - Predicting thermal performance in thermal radiation space environments requires specialized software (e.g. CR Tech Thermal Desktop, TSS, NX SST, TRASYS)
- **This section discusses methods to quickly develop thermal models of battery assemblies via SpaceClaim, TD Direct and Thermal Desktop**
- **Support material: performed two studies examining thermo-electrochemical analysis in a Thermal Desktop environment (Proof-of-Concept and Validation-of-Concept):**
  - “Thermo-electrochemical analysis of lithium ion batteries for space applications using Thermal Desktop.” Walker, W.; Ardebili, H.; JPS 2014.
  - “Thermo-electrochemical evaluation of lithium ion batteries for space applications.” Walker, W.; Yayathi, S.; Shaw, J.; Ardebili, H.; JPS 2015



# SIMULATION TECHNIQUES PART 1: THERMAL MODEL CONSTRUCTION METHODS

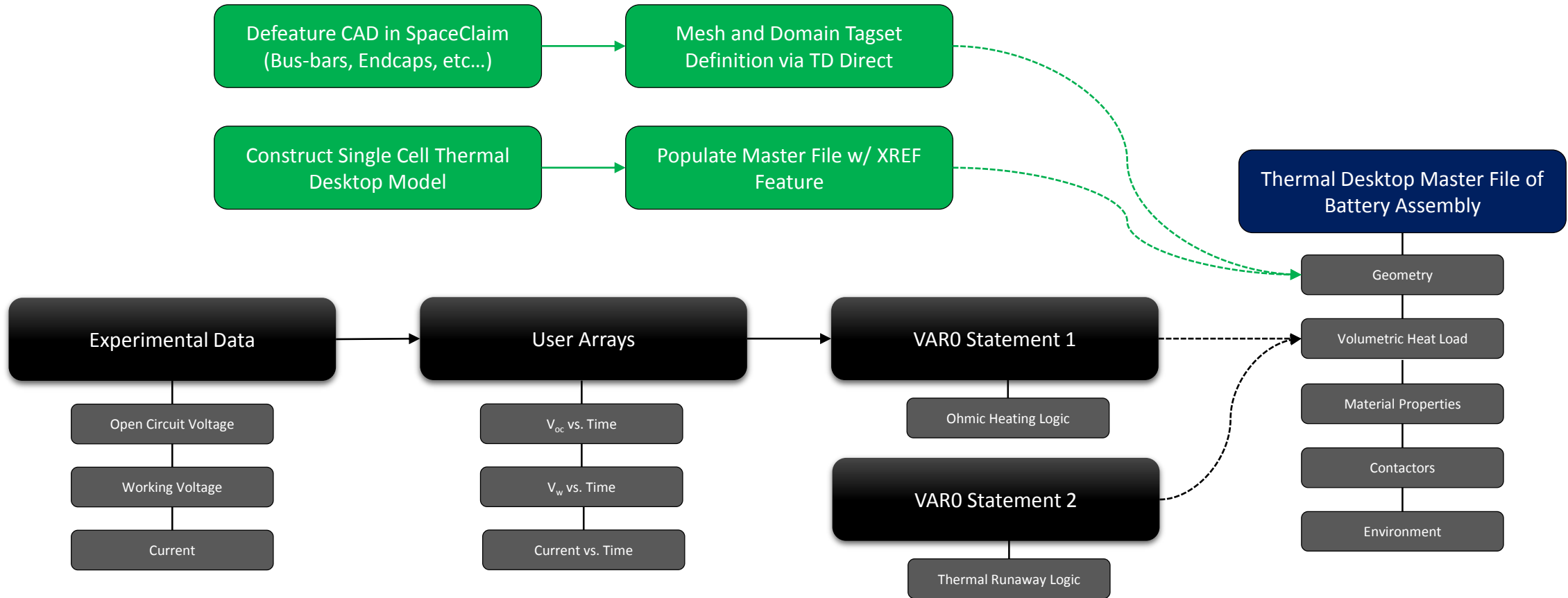


Figure adapted from "Thermo-electrochemical analysis of lithium ion batteries for space applications using Thermal Desktop." Walker, W.; Ardebili, H.; JPS 2014

# SIMULATION TECHNIQUES PART 1: THERMAL MODEL CONSTRUCTION METHODS

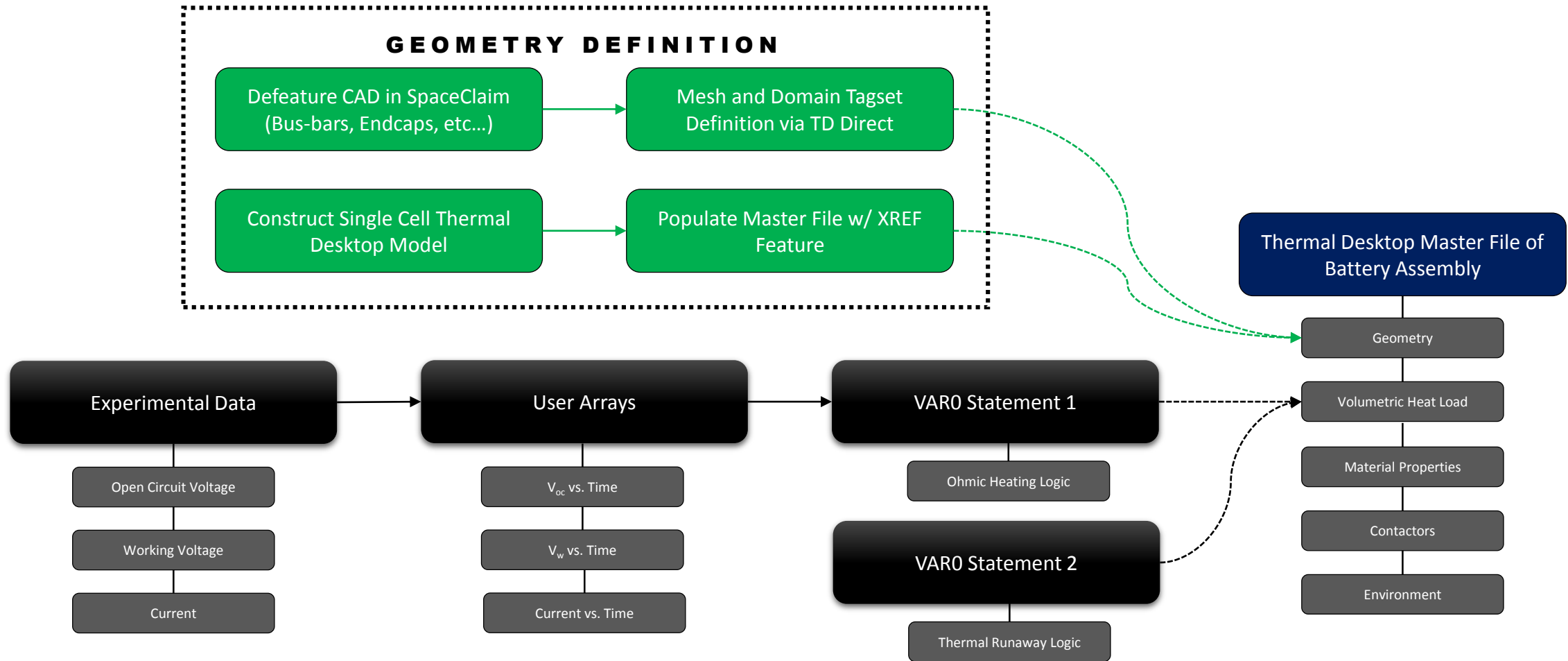
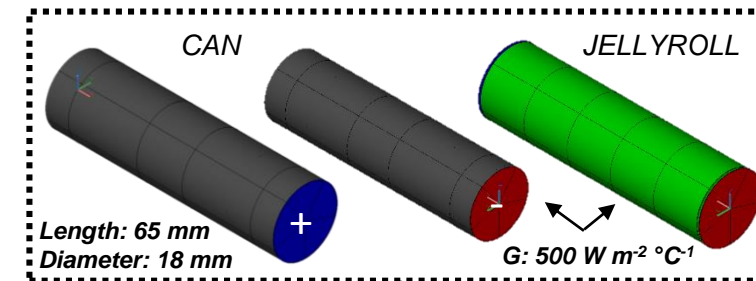


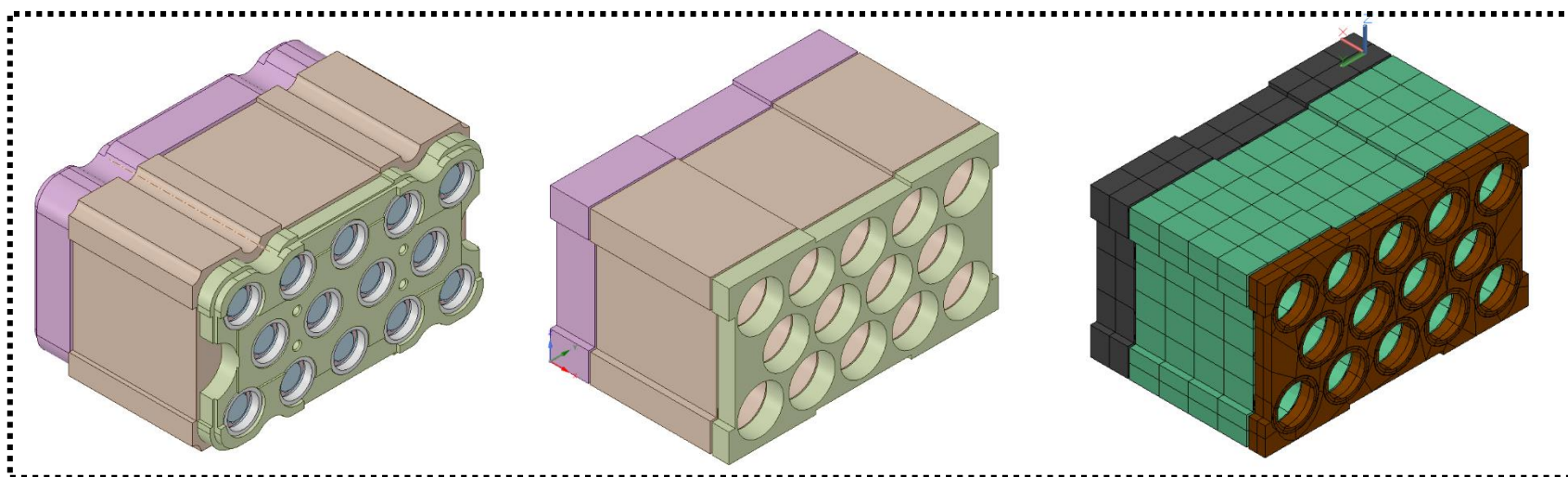
Figure adapted from "Thermo-electrochemical analysis of lithium ion batteries for space applications using Thermal Desktop." Walker, W.; Ardebili, H.; JPS 2014

## SIMULATION TECHNIQUES PART 1: THERMAL MODEL CONSTRUCTION METHODS (GEOMETRY DEFINITION)

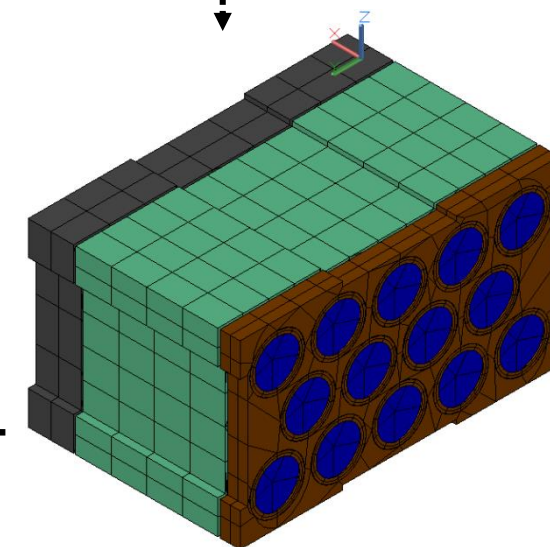
- **Example considers a bank of x14 18650 cells (similar size as AAA cell)**
- **Defeature CAD file of bank geometries via SpaceClaim and use TD Direct to provide thermal definition:**
  - Thermophysical and optical properties
  - Create a separate domain tagset for surfaces contacting the cells (contactor will be created later)
  - Separate domain tag sets should be created for any surface contacting another surface
  - Surfaces involved in radiation analysis should also be in separate
- **Create an independent Thermal Desktop model of the 18650 cell**
  - Note the distinct representation of the jellyroll AND the cell can
- **Create a master file that has a TD Direct link to the bank geometries and use the XREF feature to place the reference cell model (x14 times)**
  - Battery assemblies are developed rather quickly; these tools can help you keep up with changes



XREF



TD DIRECT



## SIMULATION TECHNIQUES PART 2: THERMAL MODEL CONSTRUCTION METHODS (GEOMETRY DEFINITION)

### ➤ Special notes on jellyroll specific heat capacity (Cp):

- The reference model of the cell should have a distinct jellyroll and a distinct cell can
- The cell can is typically made of a known material (e.g. mild steel, stainless steel or aluminum)
- The jellyroll is essentially a composite of the carbon anode, the lithium rich cathode, the electrolyte, the polymer separator and the metal current collectors; your Cp must accurately characterize the performance of these materials
- Unfortunately the vast amount of literature out there discussing the Cp of Li-ion cells is based on testing which included the cell can; hence the documents discuss the overall Cp of the cell rather than just the jellyroll
- If the jellyroll Cp is unknown, start with  $1000 \text{ J kg}^{-1} \text{ C}^{-1}$

### ➤ The image to the right demonstrates the impact that small error in Cp

### ➤ See the reference below which provides more discussion on the topic

- “Thermo-electrochemical analysis of lithium ion batteries for space applications using Thermal Desktop.” Walker, W.; Ardebili, H.; JPS 2014.

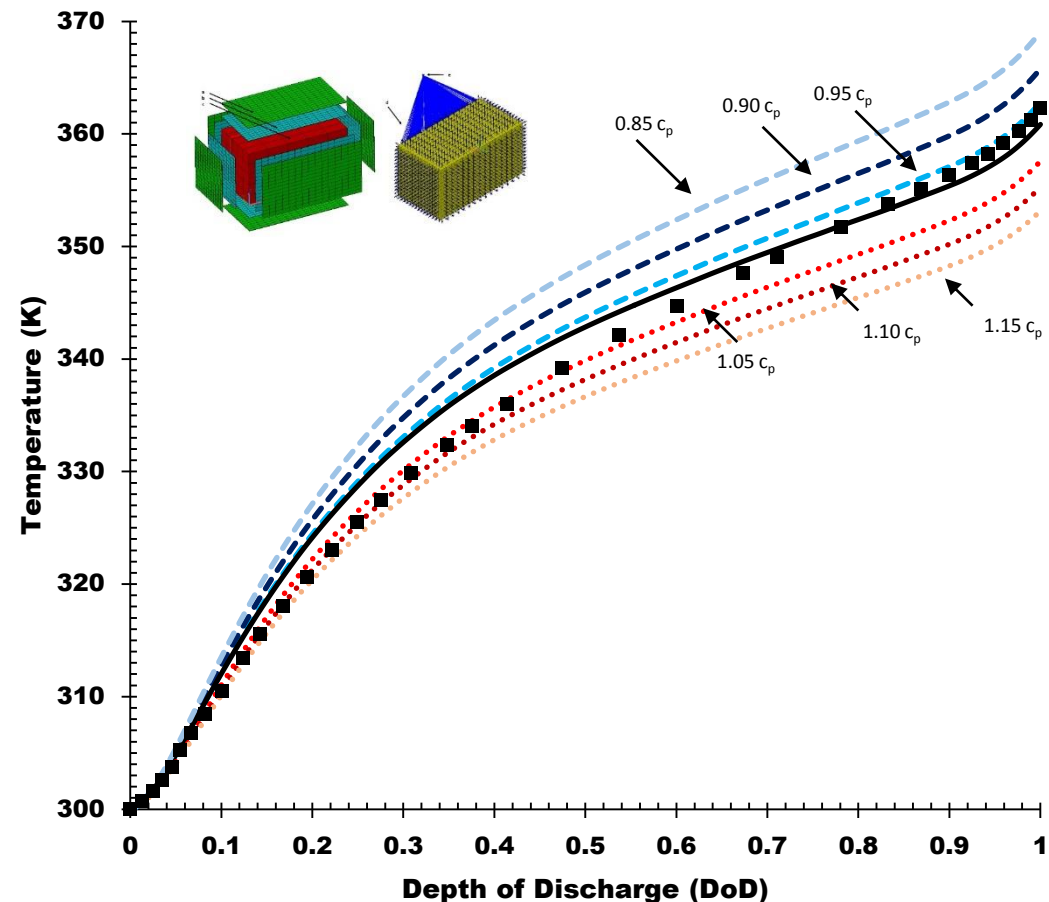


Figure adapted from “Thermo-electrochemical analysis of lithium ion batteries for space applications using Thermal Desktop.” Walker, W.; Ardebili, H.; JPS 2014

# SIMULATION TECHNIQUES PART 1: THERMAL MODEL CONSTRUCTION METHODS

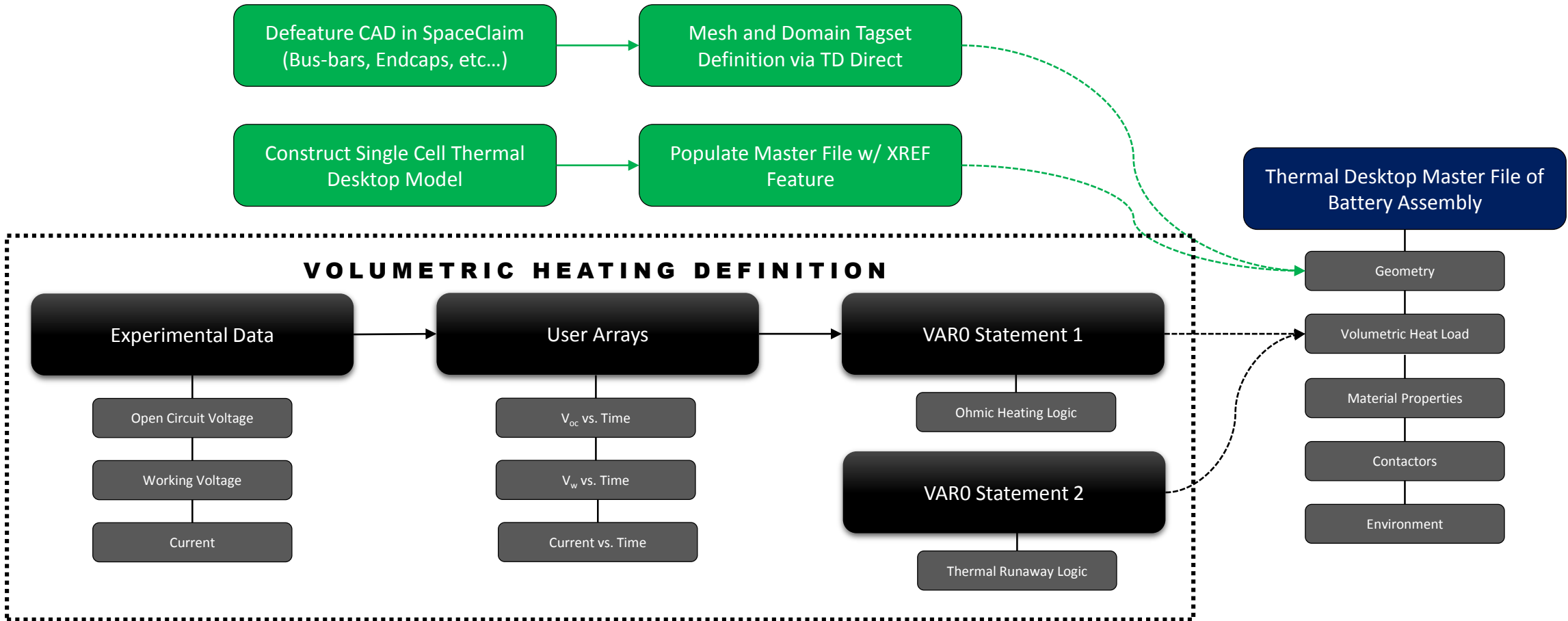


Figure adapted from "Thermo-electrochemical analysis of lithium ion batteries for space applications using Thermal Desktop." Walker, W.; Ardebili, H.; JPS 2014

# SIMULATION TECHNIQUES PART 1: THERMAL MODEL CONSTRUCTION METHODS (VOLUMETRIC HEATING DEFINITION)

- **Ohmic heat generation may be applied to as a single heat load in the master file of the battery assembly**
  - In the cell reference file, create a domain tag set that contains the jellyroll
  - In the master file, create registers for each of the variables in Bernardi's equation; we will simplify here and only use current and voltage
  - In the master file, apply "heat load to solid" and select the jellyroll domain tag set; set the value as a symbol expression of Bernardi's equation
  - In the master file, create VAR0 array interpolation or bivariate array interpolation time dependent logic objects; the array value should be defined by test
- **Running a transient simulation will now update the previously defined heat load on the jellyroll before each timestep based on the change in current, open circuit voltage and working voltage**

		<b>V<sub>oc</sub> Bivariate Array</b>					<b>V<sub>w</sub> Bivariate Array]</b>					
		↓					↓					
		-45°C	-25°C	0°C	+25°C	+45°C						
<b>Q<sub>JELL</sub> = Current x</b>	0min	#	#	#	#	#	0min	#	#	#	#	#
	10min	#	#	#	#	#	10min	#	#	#	#	#
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## SIMULATION TECHNIQUES PART 1: THERMAL MODEL CONSTRUCTION METHODS (VOLUMETRIC HEATING DEFINITION)

- **Disclaimer: these simulations are still in development and are not test correlated, but do demonstrate the capability we will gain once completed**
- **Thermal runaway logic here considers:**
  - Jellyroll trigger temperature (**TTRIG**)
  - Length of the runaway event (**TEVENT**)
  - Energy released per second (**QEVENT**)
  - Ensures runaway only happens once (**RUNAWAY**)
  - Deactivates exterior heater (**END\_TRIGGER**)
- **It is challenging, but possible, to establish logic that triggers runaway on a per cell basis as a function of temperature that will only occur once in the life of the cell**
- **This logic does NOT include:**
  - Boiling and venting of the electrolyte, which affect the general heat rate profile
  - Designation of fraction of energy through the sides of the cell, the top and in the ejecta/gas; assumes all heat is generated in the jellyroll
- **Ultimate goal when developing this basic code was to use Thermal Desktop for battery design certification**
  - Pre-determine the thermal environment a permanently mounted Li-ion battery must operate in and design to that environment
  - Determine attitudes and environments which would induce thermal runaway and propagation
  - **A good question from TFAWS; “what does the propagation scenario look like if you have an environmentally induced failure – aren’t all of your cells close to the trigger temperature rather than just a single cell?”**

### FSTART

C find submodel reference ID

```
call modtrn('jell',mtest)
```

C loop through all diffusion nodes in the submodel

C assumes nodes are sequentially numbered

```
do itest = 1, nmdif(mtest)
```

C look up node storage location

```
call nodtrn('jell',itest,mtest)
```

C perform runaway logic

```
if ((T(mtest) .ge. TTRIG) .and. (runaway .ge. 0)) then
```

```
  if (runaway .eq. 0) then
```

```
    end_trigger = TIMEN + TEVENT
```

```
    runaway = 1
```

```
  end if
```

```
  if (TIMEN .le. end_trigger) then
```

C use capacitance fraction to proportion the heat load

C battery\_mCp can be calculated in advance

```
  Q(mtest) = Q(mtest) + QEVENT*C(mtest)/JELLMCP
```

```
  else
```

```
  Q(mtest) = Q(mtest) + 0.
```

```
  runaway = -1
```

```
  end if
```

```
end if
```

```
end do
```

### FSTOP

## SIMULATION TECHNIQUES PART 1: THERMAL MODEL CONSTRUCTION METHODS (VOLUMETRIC HEATING DEFINITION)

### ➤ Can we use the **SINDA DIFFEQ** statement to solve the models discussed on [slide 18](#) instead?

- Answer: It is possible, but there are some limitations due to timestep control because some of the terms approach zero

<pre> C OPERATIONS  CALL DIFFEQ1I( 1, Xcati, DXcDT)  CALL DIFFEQ1I( 2, Xseii, DXsDT)  CALL DIFFEQ1I( 3, Xani, DXaDT)  CALL DIFFEQ1I( 4, Z0, DZDT)  CALL DIFFEQ1I( 5, SoCi, DSoCDT)  C SYMBOL MANAGER  Qsei = man*Hsei*dXsdt  Qec = -(mcat+man)*Hec*dSoCdt  Qcat = mcat*Hcat*dXcDT  Qan = man*Han*dXandT           </pre>	<pre> C VAR2  CALL DIFFEQ1( 1, Xcat, 1.0, Fcat*(1-Xcat)*EXP(- Ecat/(Kb*JELL.T1)),0.0)  DXcDT = Fcat*Xcat*(1-Xcat)*EXP(-Ecat/(Kb*JELL.T1))  CALL DIFFEQ1( 2, Xsei, 1.0, -Fsei*EXP(-Esei/(Kb*JELL.T1)),0.0)  DXsDT = -Fsei*Xsei*EXP(-Esei/(Kb*JELL.T1))  CALL DIFFEQ1( 3, Xan, 1.0, -Fan*EXP(-Ean/(Kb*JELL.T1))*EXP(- Z/Z0),0.0)  DXaDT = -Fan*Xan*EXP(-Ean/(Kb*JELL.T1))*EXP(-Z/Z0)  CALL DIFFEQ1( 4, Z, 1.0, 0.0, Xan*Fan*EXP(-Ean/(Kb*JELL.T1))*EXP(- Z/Z0))  DZDT = Xan*Fan*EXP(-Ean/(Kb*JELL.T1))*EXP(-Z/Z0)  CALL DIFFEQ1( 5, SoC, 1.0, 0.0, -Fec*(1-Xcat)*Xan*exp(- Eec/(Kb*JELL.T1))+(DXaDT-DXcDT)*SoC)  DSoCDT = -Fec*(1-Xcat)*Xan*exp(-Eec/(Kb*JELL.T1))+ (DXaDT-DXcDT)*SoC  C VAR0           </pre>
--	--

**Credit: Lewis Jones (ES3 Intern)**

# SIMULATION TECHNIQUES PART 1: THERMAL MODEL CONSTRUCTION METHODS

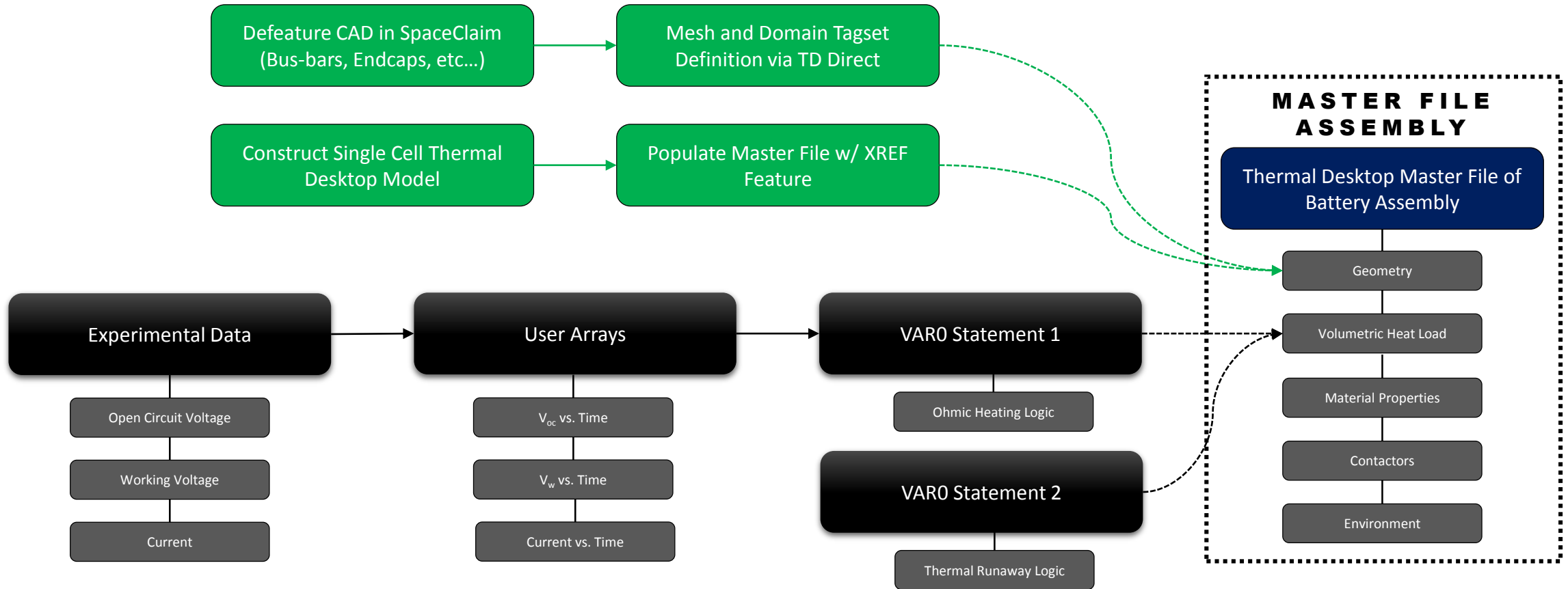
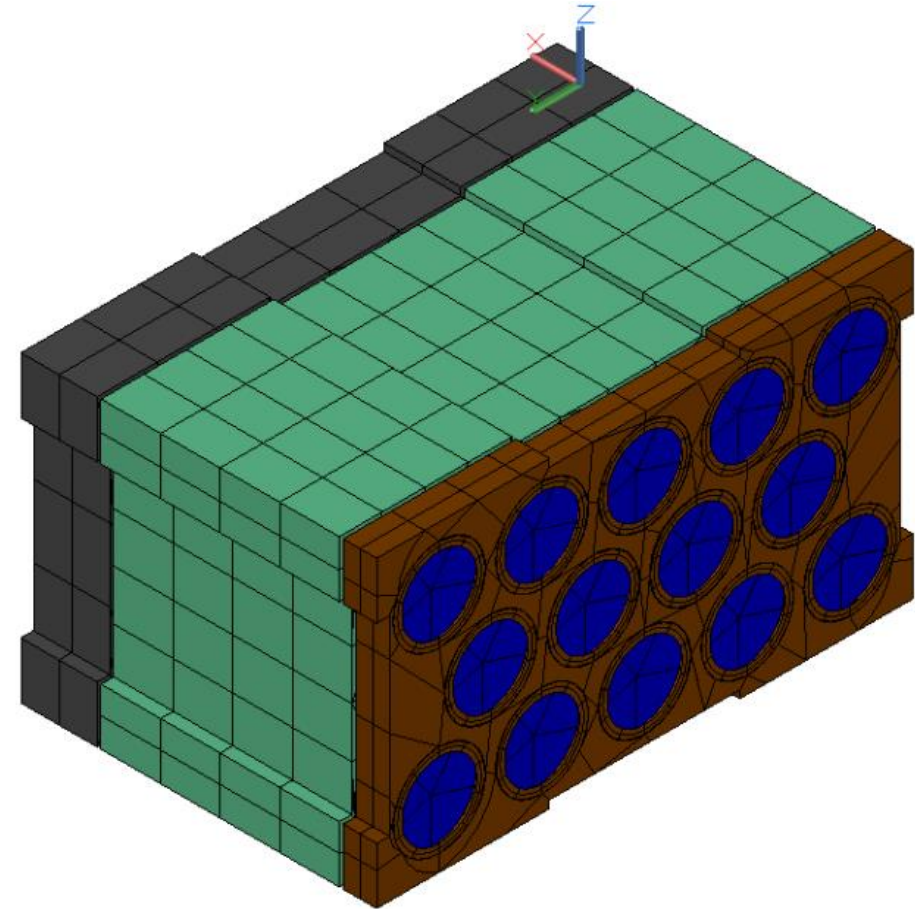


Figure adapted from "Thermo-electrochemical analysis of lithium ion batteries for space applications using Thermal Desktop." Walker, W.; Ardebili, H.; JPS 2014

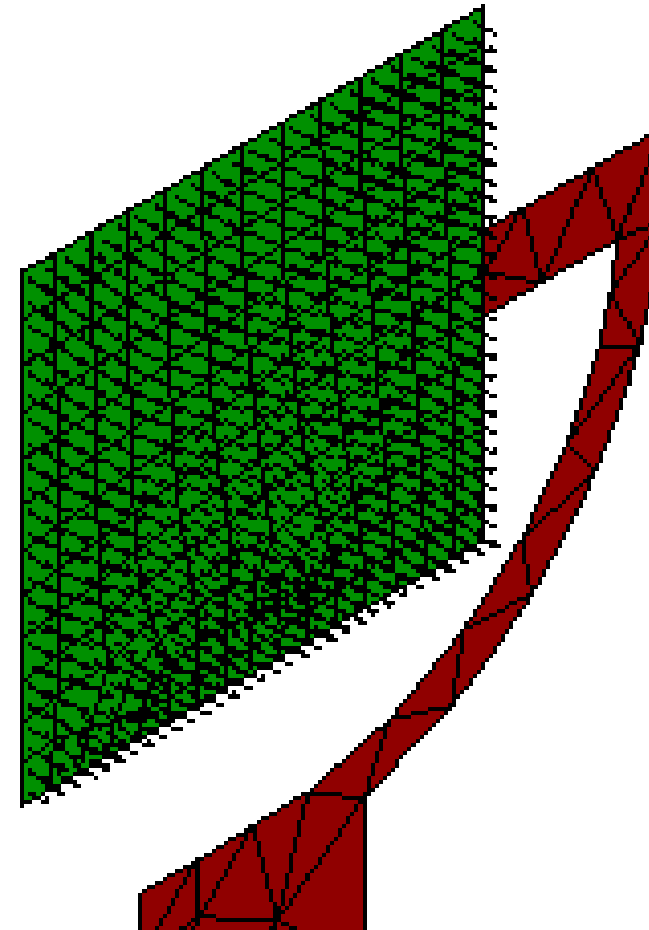
## SIMULATION TECHNIQUES PART 2: THERMAL MODEL CONSTRUCTION METHODS (MASTER FILE ASSEMBLY)

- **The geometries and heat loads are defined in the master file by following the steps listed in the previous slides**
- **Create contactors between the bank geometries and the cell geometries via Domain Tagsets:**
  - **DTS\_CELL\_TO\_FOAM** TO **DTS\_FOAM\_TO\_CELL**
  - **DTS\_CELL\_TO\_POS\_ENDCAP** TO **DTS\_POS\_ENDCAP\_TO\_CELL**
  - **DTS\_CELL\_TO\_NEG\_ENDCAP** TO **DTS\_NEG\_ENDCAP\_TO\_CELL**
- **Make sure that all material properties used via TD Direct or used in the single 18650 cell reference file are recreated in the Master File thermophysical property and optical property databases**
- **Note the anisotropy of the thermal conductivity for the jellyroll due to the layers:**
  - Cylindrical Cell: 28 (height) / 28 (angular) / 3 (radial)  $\text{W m}^{-1} \text{ } ^\circ\text{C}^{-1}$
  - Prismatic Cell: 28 (x, y) / 3 (z – i.e. thickness)  $\text{W m}^{-1} \text{ } ^\circ\text{C}^{-1}$
- **Define the convection and radiation environment:**
  - Note that any TD Direct or XREF surface involved with the environment requires the definition of Domain Tagsets for the interactive surfaces



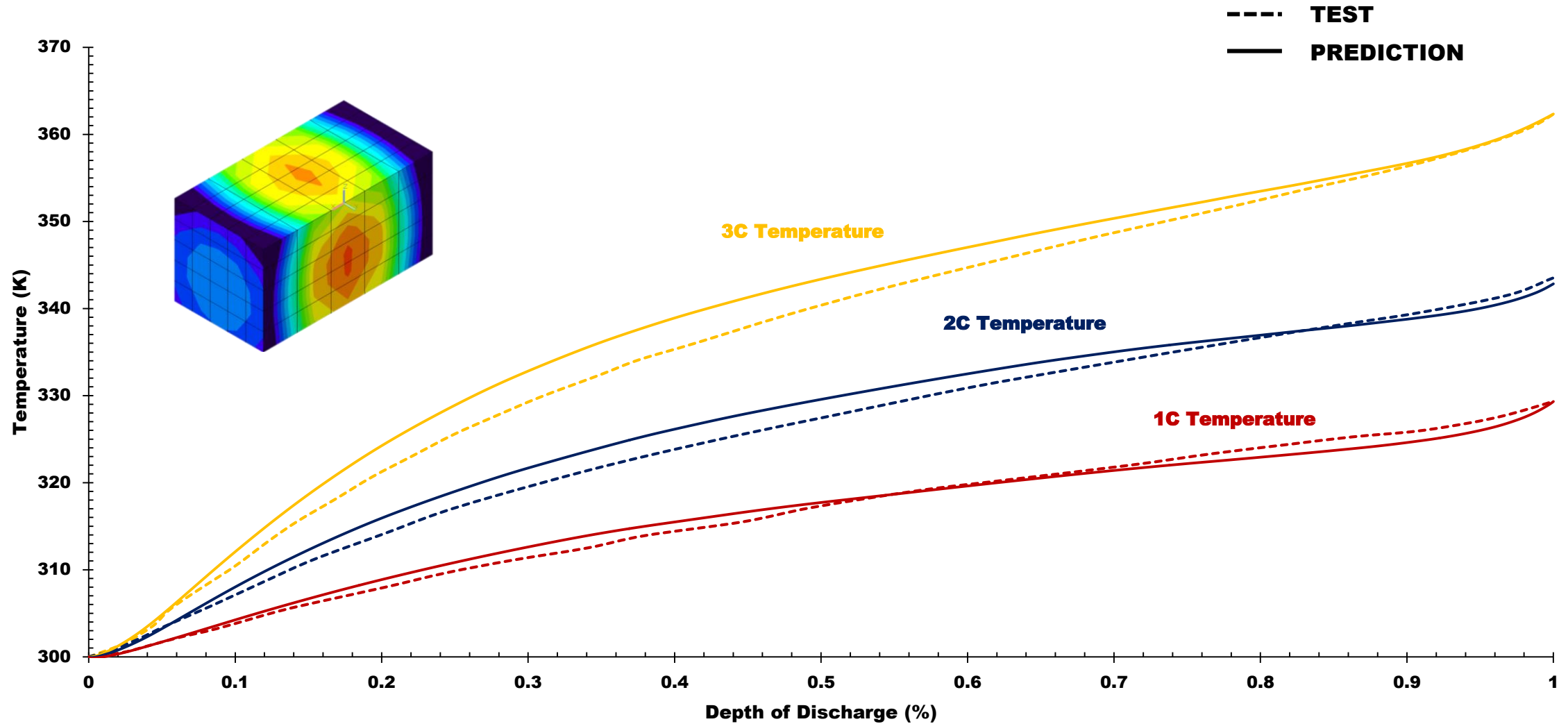
## **SIMULATION TECHNIQUES PART 1:** THERMAL MODEL CONSTRUCTION METHODS (MASTER FILE ASSEMBLY)

- **Special notes on creating contact in the master file between the reference cell file and the TD Direct bank geometry import:**
  - Use TD Direct to create domain tag sets of areas in contact for the bank geometries
  - Manually create domain tag sets of areas in contact in the cell reference file
  - Create a contactor in the master file which references both domain tag sets
- **Examples of useful areas to have domain tagsets:**
  - Top/bottom of cell in the cell reference model
  - Busbar tabs that will connect to the top/bottom of the cells
  - Outside surfaces of the cell that will be in contact with the endcaps and interstitial materials
  - Inside surfaces of endcaps and interstitial materials that will be in contact with the cell
  - Locations of contact for the bank geometries
- **Domain tag sets can also be used to identify areas for special cases; e.g. application of a patch heater to induce thermal runaway**



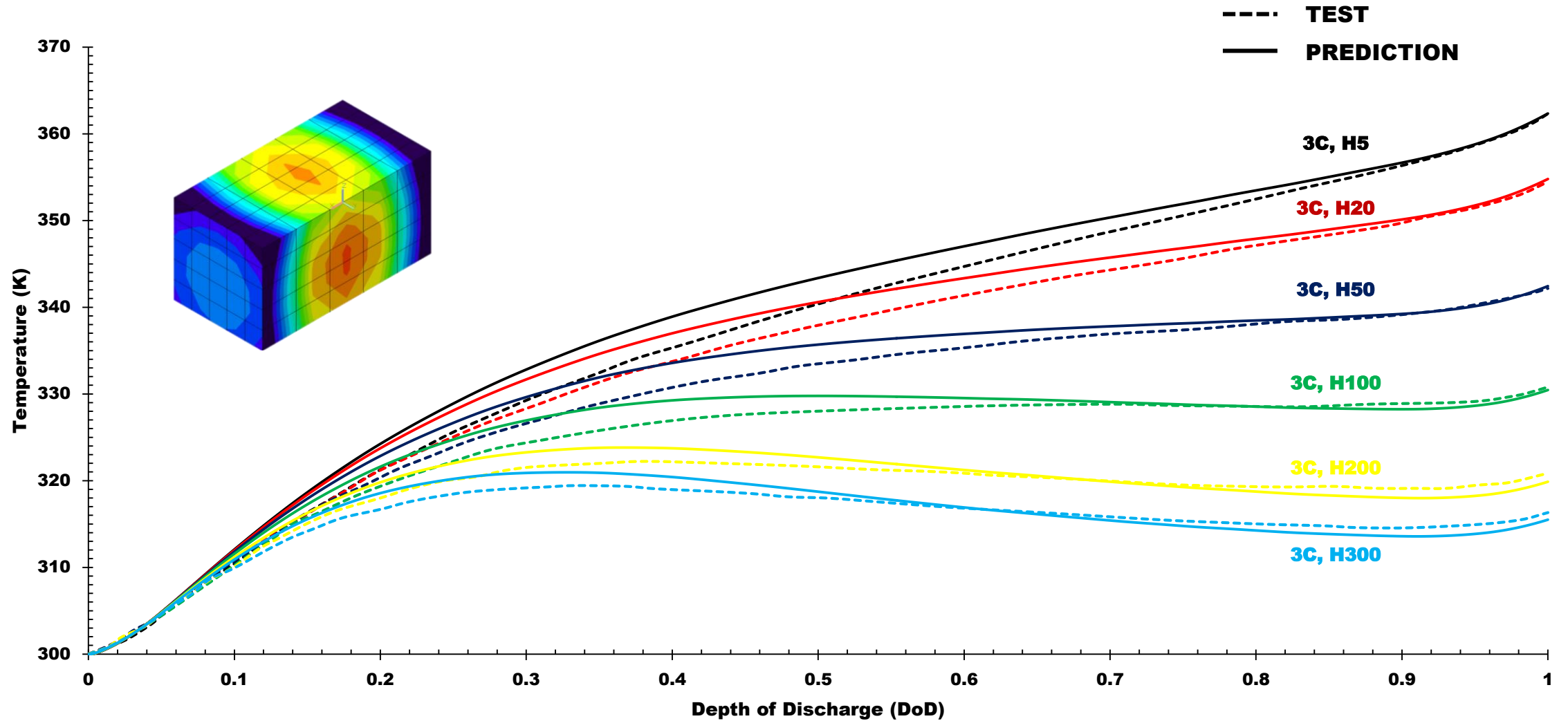
# **SECTION 5: SIMULATION TECHNIQUES PART 2: EXAMPLE ANALYSIS RESULTS**

## SIMULATION TECHNIQUES PART 2: LARGE BATTERY ASSEMBLY ANALYSIS RESULTS (DISCHARGE)



Comparison of TD-S results, Chen's results and experimental results for 1.0C-3.0C discharge rates in a natural convection environment [47-48]

## SIMULATION TECHNIQUES PART 2: LARGE BATTERY ASSEMBLY ANALYSIS RESULTS (DISCHARGE)



Comparison of TD-S results, Chen's results and experimental results for 3.0C discharge rate in varied forced convection environments (20-300 W m<sup>-2</sup> °C<sup>-1</sup>) [47-48]



# SIMULATION TECHNIQUES PART 2: SINGLE CELL ANALYSIS RESULTS (CHARGE)

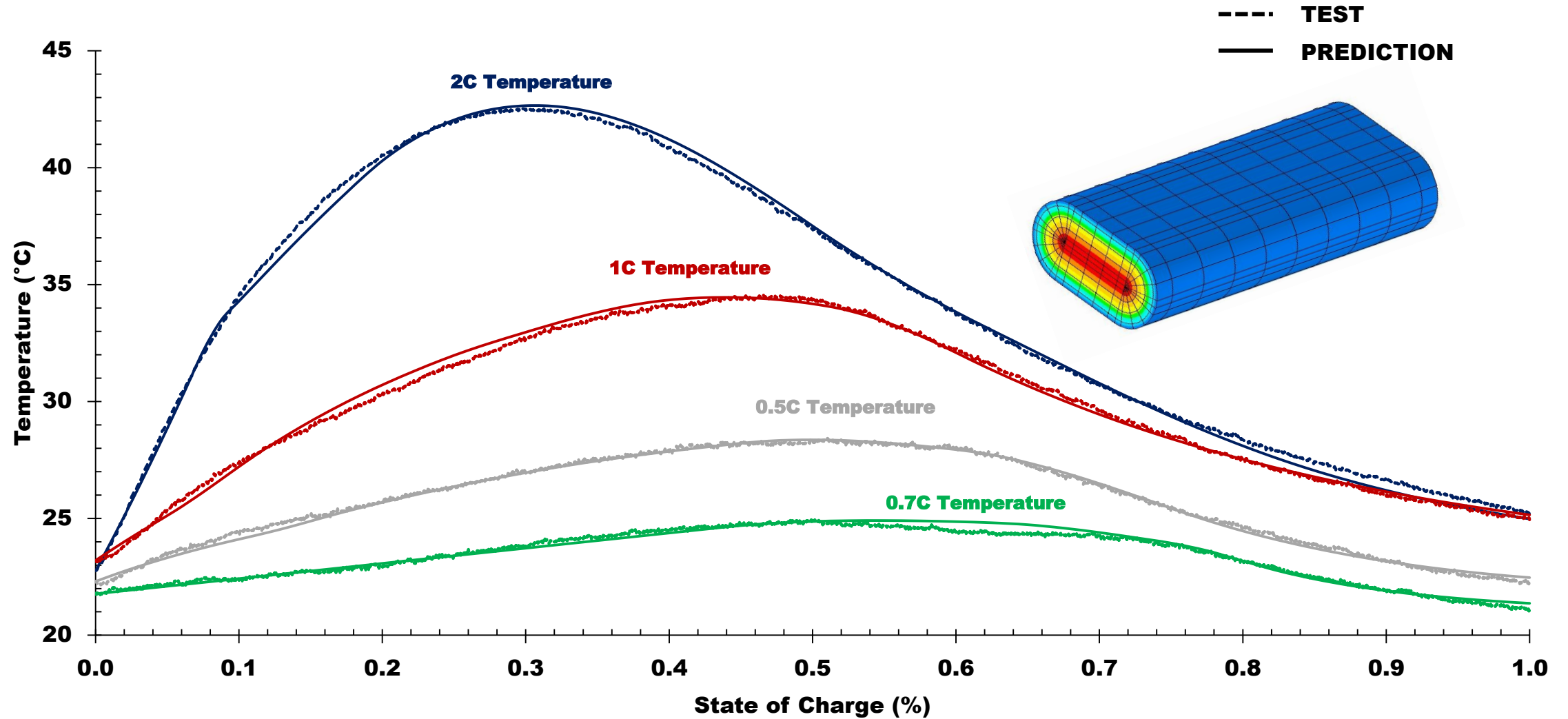
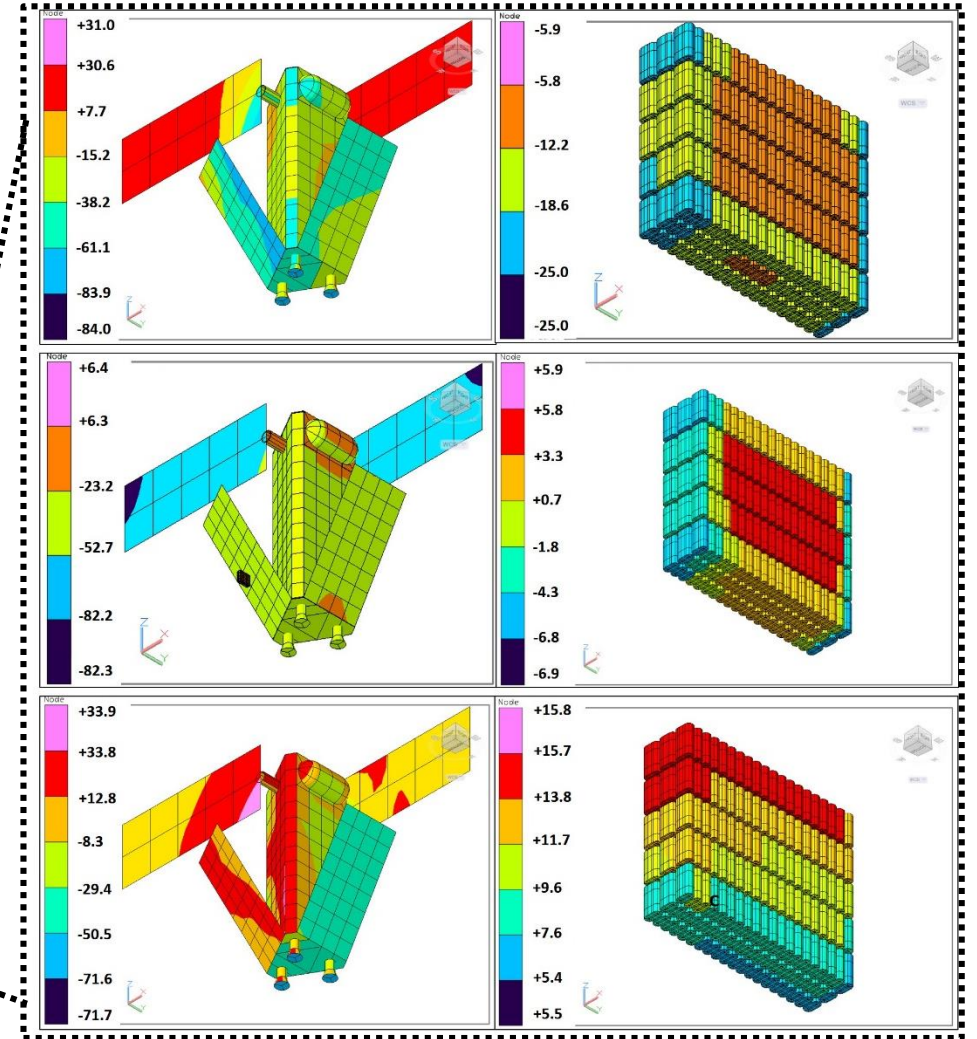
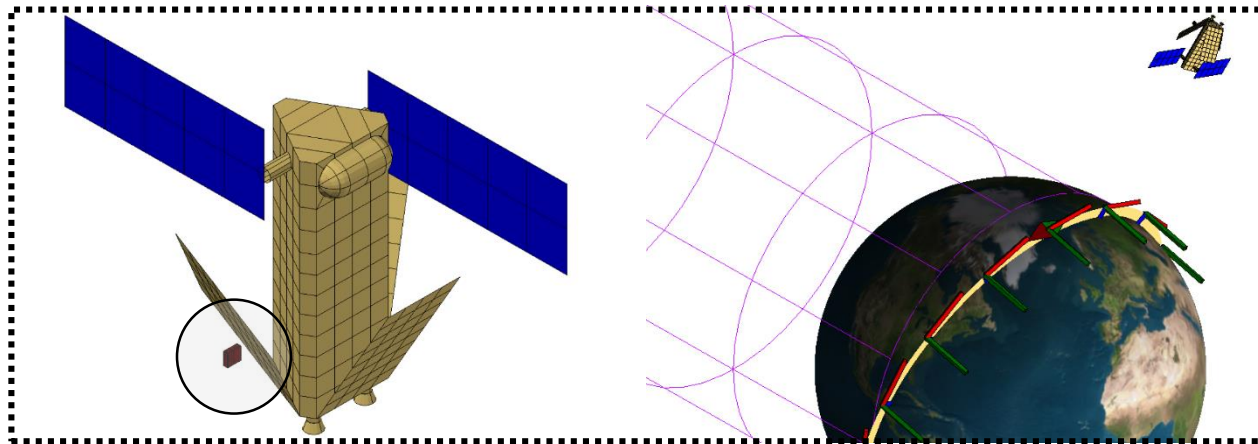
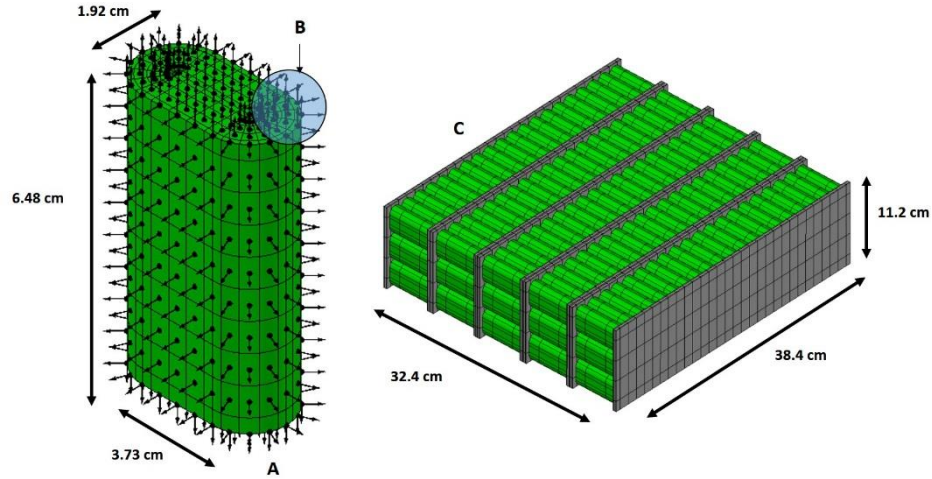


Image adapted from "Thermo-electrochemical evaluation of lithium ion batteries for space applications." Walker, W.; Yayathi, S.; Shaw, J.; Ardebili, H.; (JPS 2015)

# SIMULATION TECHNIQUES PART 2: SINGLE CELL ANALYSIS RESULTS (CHARGE)



R2 300 cell system level model simulated (a) exterior to an example satellite in a (b) -75 beta orbit, (c) 0 beta orbit and (d) +75 beta orbit [TBD]

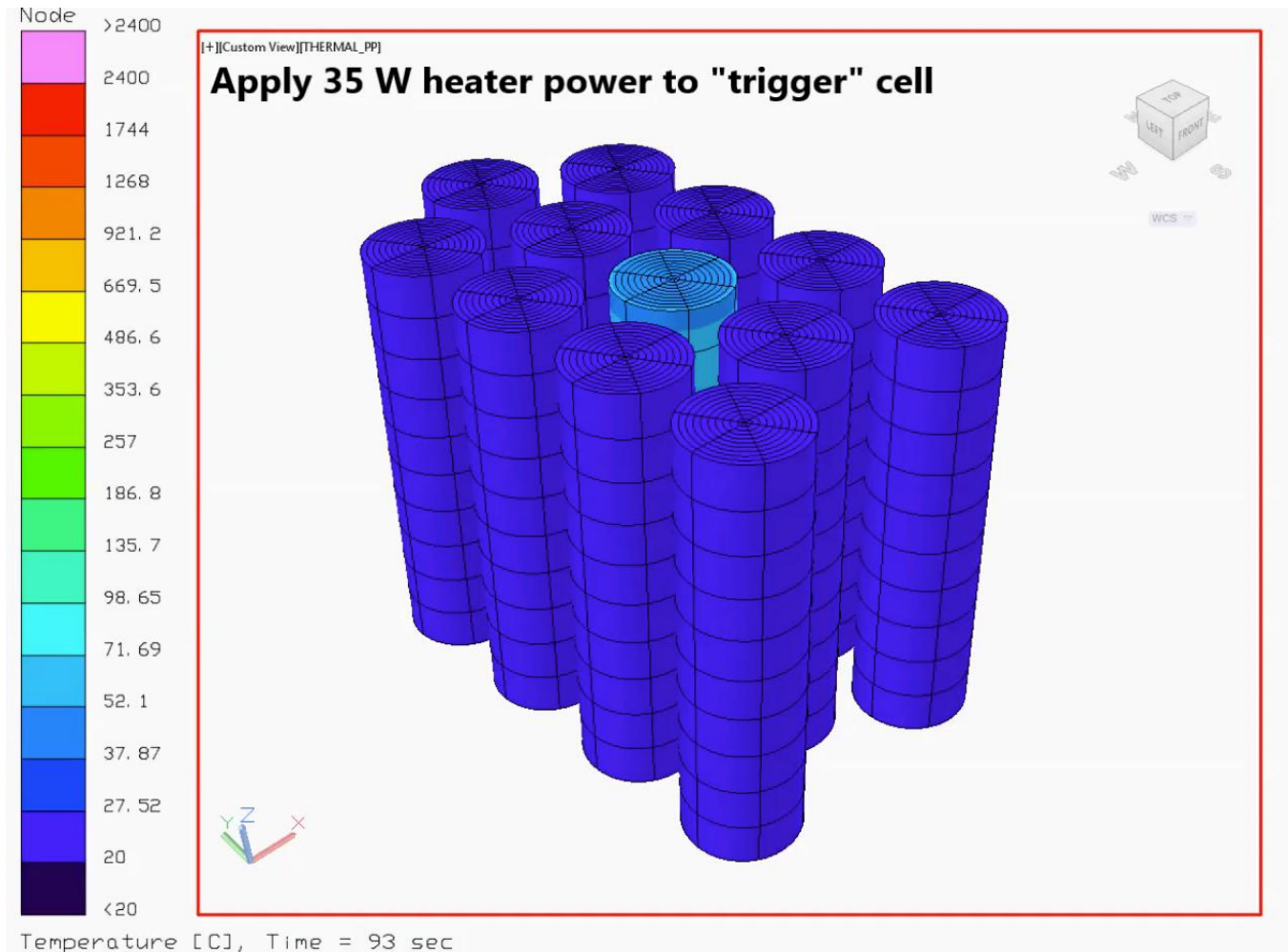
## SIMULATION TECHNIQUES PART 2: THERMAL RUNAWAY ANALYSIS RESULTS (USER DEFINED HEATING)

### FSTART

```

C find submodel reference ID
  call modtrn('jell',mtest)
C loop through all diffusion nodes in the submodel
C assumes nodes are sequentially numbered
  do itest = 1, nmdif(mtest)
C look up node storage location
  call nodtrn('jell',itest,ntest)
C perform runaway logic
  if ((T(ntest) .ge. TTRIG) .and. (runaway .ge. 0)) then
    if (runaway .eq. 0.) then
      end_trigger = TIMEN + TEVENT
      runaway = 1
    end if
    if (TIMEN .le. end_trigger) then
C use capacitance fraction to proportion the heat load
C battery_mCp can be calculated in advance
      Q(ntest) = Q(ntest) + QEVENT*C(ntest)/JELLMCP
    else
      Q(ntest) = Q(ntest) + 0.
      runaway = -1
    end if
  end if
end do
  
```

### FSTOP



## SIMULATION TECHNIQUES PART 2: THERMAL RUNAWAY ANALYSIS RESULTS (PHYSICS DEFINED HEATING)

### C OPERATIONS

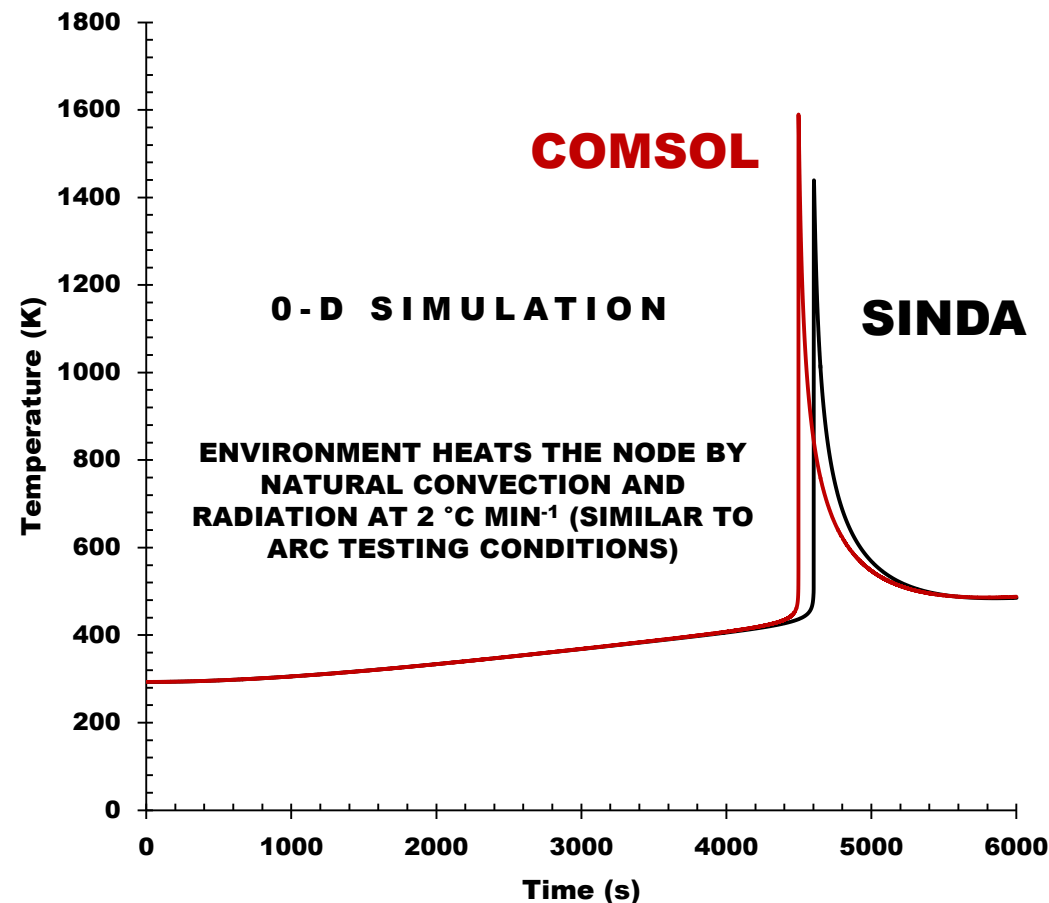
```
CALL DIFFEQ1I( 1, Xcati, DXcDT)
CALL DIFFEQ1I( 2, Xseii, DXsDT)
CALL DIFFEQ1I( 3, Xani, DXaDT)
CALL DIFFEQ1I( 4, Z0, DZDT)
CALL DIFFEQ1I( 5, SoCi, DSoCDT)
```

### C SYMBOL MANAGER

```
Qsei = man*Hsei*dXsdt
Qec = -(mcat+man)*Hec*dSoCdt
Qcat = mcat*Hcat*dXcDT
Qan = man*Han*dXandT
```

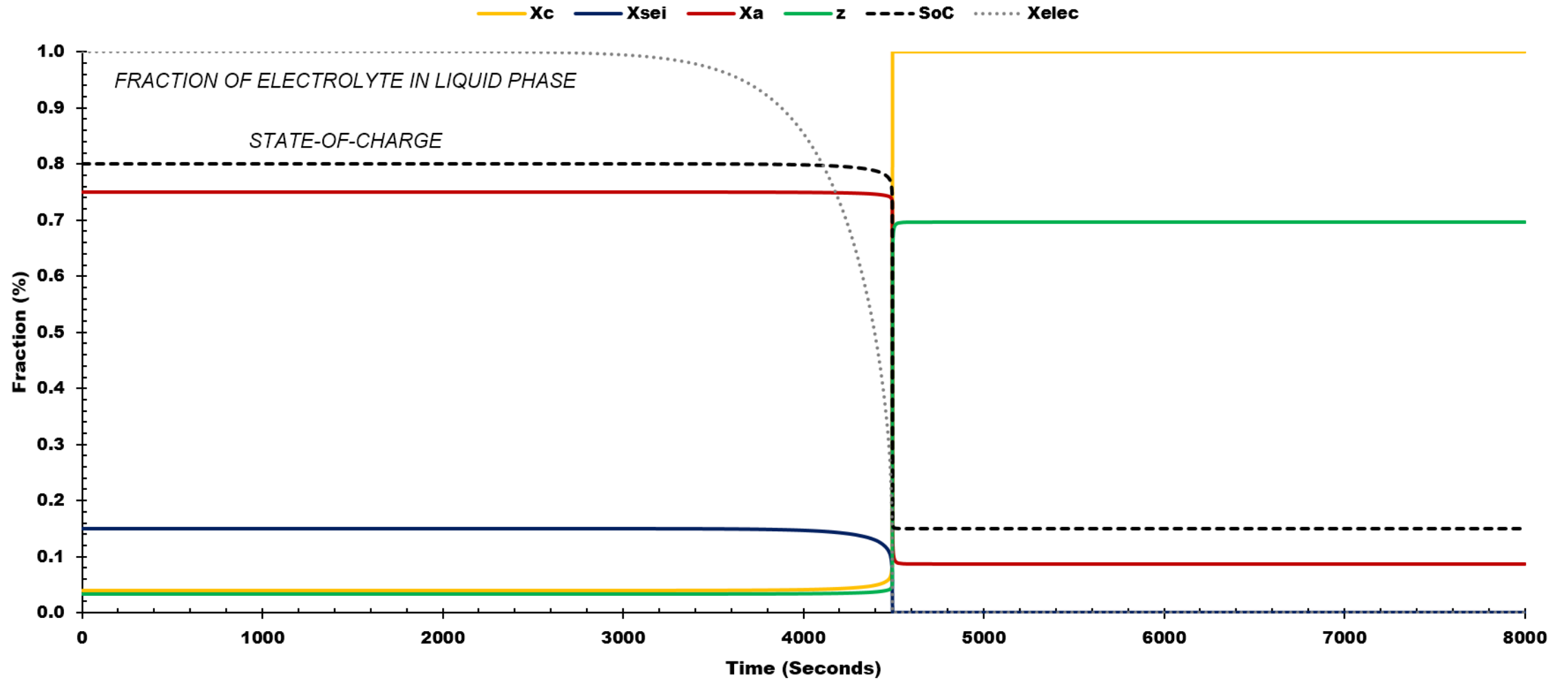
### C VAR2

```
CALL DIFFEQ1( 1, Xcat, 1.0, Fcat*(1-Xcat)*EXP(-Ecat/(Kb*JELL.T1)),0.0)
DXcDT = Fcat*Xcat*(1-Xcat)*EXP(-Ecat/(Kb*JELL.T1))
CALL DIFFEQ1( 2, Xsei, 1.0, -Fsei*EXP(-Esei/(Kb*JELL.T1)),0.0)
DXsDT = -Fsei*Xsei*EXP(-Esei/(Kb*JELL.T1))
CALL DIFFEQ1( 3, Xan, 1.0, -Fan*EXP(-Ean/(Kb*JELL.T1))*EXP(-Z/Z0),0.0)
DXaDT = -Fan*Xan*EXP(-Ean/(Kb*JELL.T1))*EXP(-Z/Z0)
CALL DIFFEQ1( 4, Z, 1.0, 0.0, Xan*Fan*EXP(-Ean/(Kb*JELL.T1))*EXP(-Z/Z0))
DZDT = Xan*Fan*EXP(-Ean/(Kb*JELL.T1))*EXP(-Z/Z0)
CALL DIFFEQ1( 5, SoC, 1.0, 0.0, -Fec*(1-Xcat)*Xan*exp(-Eec/(Kb*JELL.T1))+(DXaDT-DXcDT)*SoC)
DSoCDT = -Fec*(1-Xcat)*Xan*exp(-Eec/(Kb*JELL.T1))+(DXaDT-DXcDT)*SoC
C VAR0
```



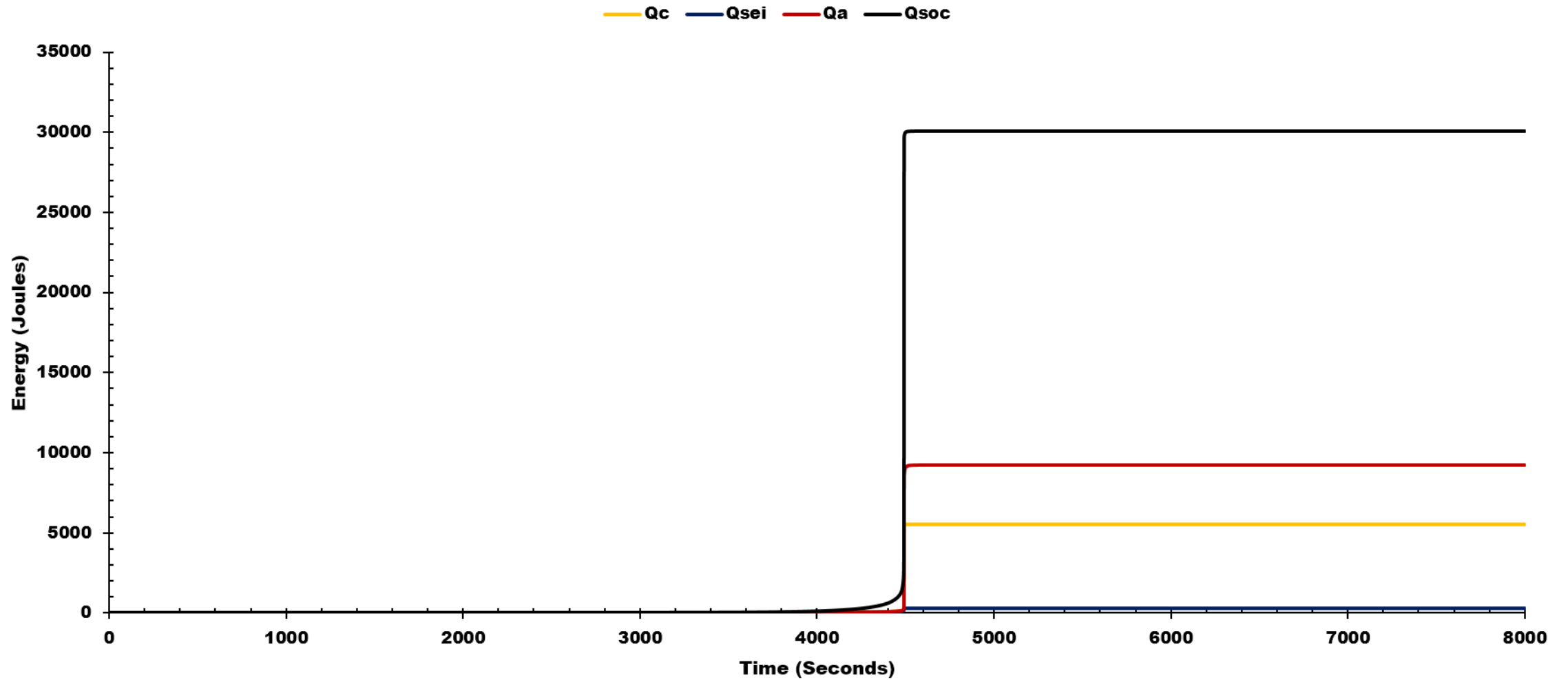
Simulations based on mathematic models developed by Richard and Dahn, Hatchard et. al., Kim et. al. and Coman et. al. [67-70].

## SIMULATION TECHNIQUES PART 2: THERMAL RUNAWAY ANALYSIS RESULTS (PHYSICS DEFINED HEATING)



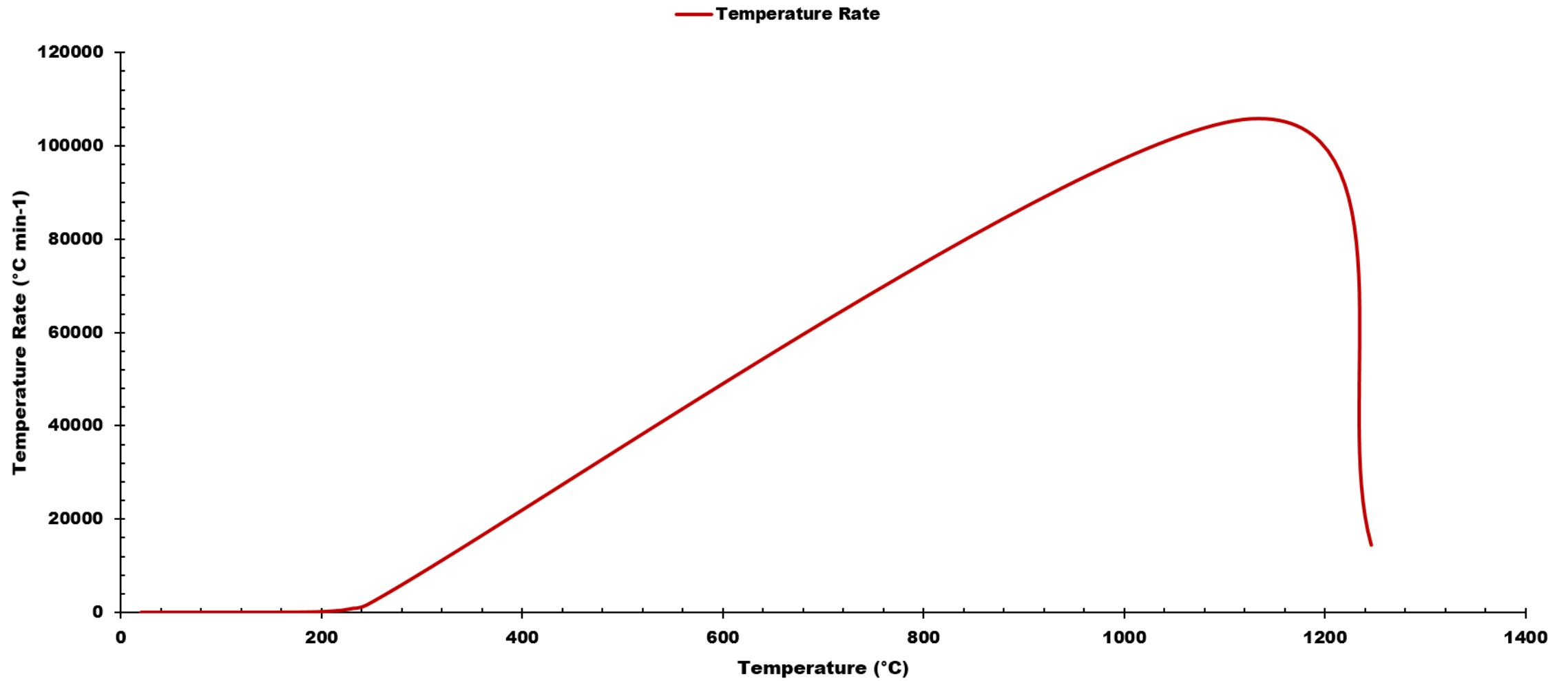
Simulations based on mathematic models developed by Richard and Dahn, Hatchard et. al., Kim et. al. and Coman et. al. [67-70].

## SIMULATION TECHNIQUES PART 2: THERMAL RUNAWAY ANALYSIS RESULTS (PHYSICS DEFINED HEATING)



Simulations based on mathematic models developed by Richard and Dahn, Hatchard et. al., Kim et. al. and Coman et. al. [67-70].

## SIMULATION TECHNIQUES PART 2: THERMAL RUNAWAY ANALYSIS RESULTS (PHYSICS DEFINED HEATING)



Simulations based on mathematic models developed by Richard and Dahn, Hatchard et. al., Kim et. al. and Coman et. al. [67-70].

## **WRAP-UP AND ACKNOWLEDGEMENTS**

- **Course covered the fundamentals of Li-ion batteries, heating mechanisms and some simulation techniques; the recording of this session will be available through the NESC Engineering Academy**
- **Another course will be offered in the near future by Bruce Drolen (Boeing) through the NESC Engineering Academy that provides a more extensive focus thermal runaway**
- **Special thanks to the NASA JSC Engineering Directorate (EA), Structural Engineering Division (ES) and Thermal Design Branch (ES3) Management**
- **Special thanks to Steve Rickman and Dr. Christopher Iannello (NASA Engineering and Safety Center)**
- **Special thanks to Dr. Eric Darcy (NASA JSC EP)**
- **Special thanks to Dr. Haleh Ardebili (University of Houston)**



# QUESTIONS?

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