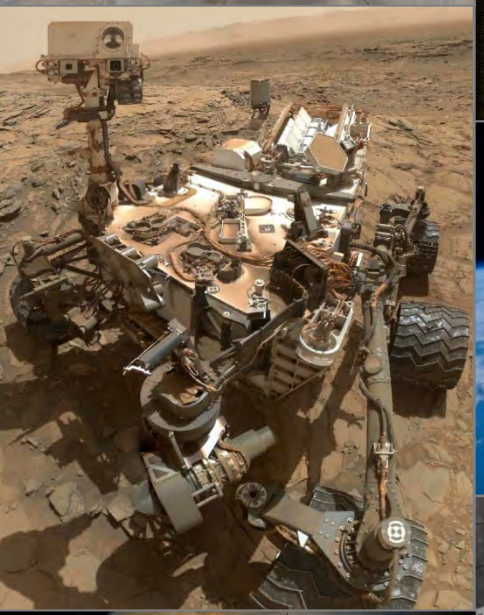
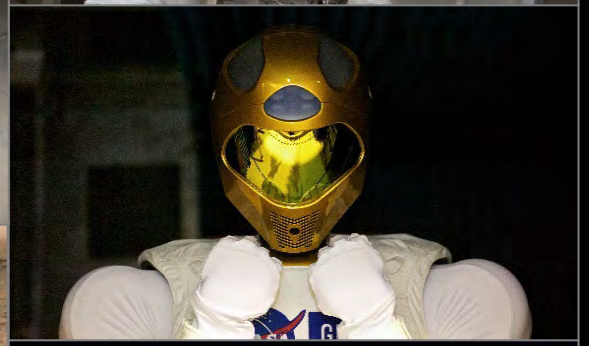
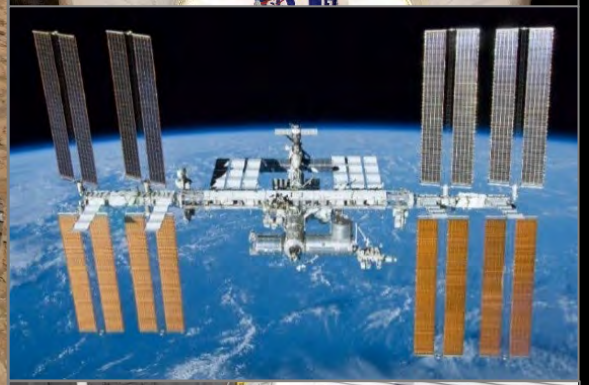





SHORT COURSE ON LITHIUM-ION BATTERIES: FUNDAMENTAL CONCEPTS, BATTERY SAFETY, AND MODELING TECHNIQUES

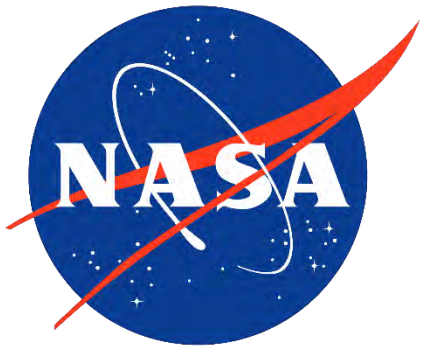
William Walker, Ph.D.
william.walker@nasa.gov

ABOUT THIS COURSE

- **This short course is designed to educate participants in the following areas:**
  - Fundamental concepts regarding Lithium-ion (Li-ion) batteries and how they work
  - Heat generation mechanisms for nominal operations and during thermal runaway
  - Battery safety, best handling practices, abuse testing, and lessons learned
  - Practical model construction techniques and example simulation results for both nominal operations and for thermal runaway
- **In general, this short course focuses on Li-ion batteries from a thermo-electrochemical perspective**
- **Although extensive, this short course is not comprehensive and should not be used as a replacement for consulting with your resident battery experts for specific advice and design guidelines**

ABOUT THE INSTRUCTOR

- **B.S. Mechanical Engineering from West Texas A&M University**
- **Ph.D. Materials Science and Engineering from the University of Houston**
- **Dissertation research primarily focused on the energy generated due to thermal runaway**
- **Civil Servant at the National Aeronautics and Space Administration (NASA) Johnson Space Center (JSC)**
  - Employed by NASA JSC for nearly 10 years
  - Specialized in Lithium-ion (Li-ion) batteries for 6 years
  - Supported battery safety related tasks for the Orion Multi-Purpose Crew Vehicle (MPCV), the International Space Station (ISS), old and new space suits, and other various applications that require Li-ion technology
  - Recent focus has been on the development of fractional thermal runaway calorimetry techniques (more on that later…)

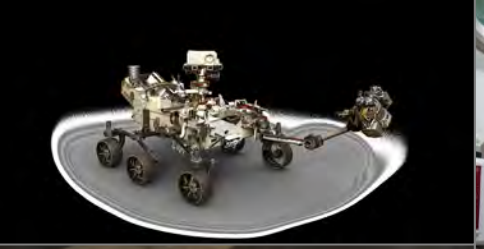


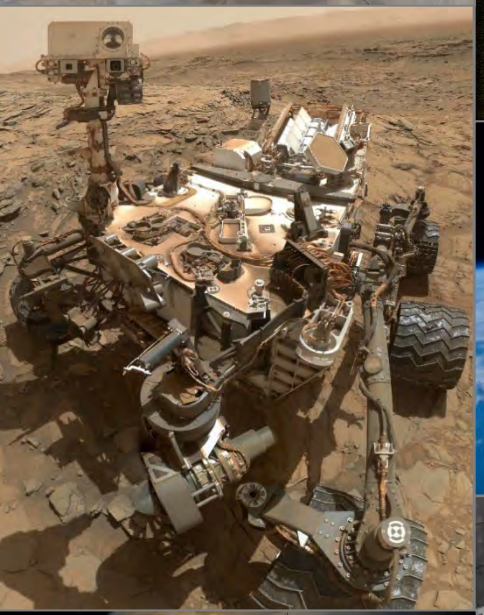


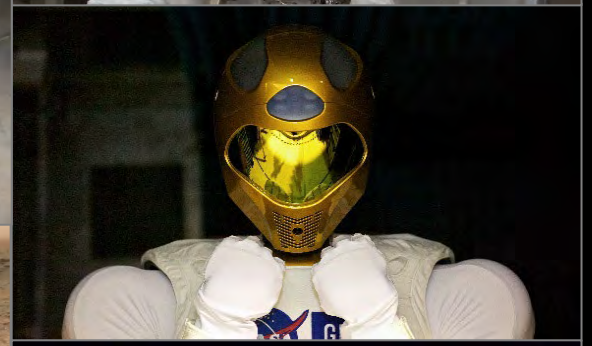
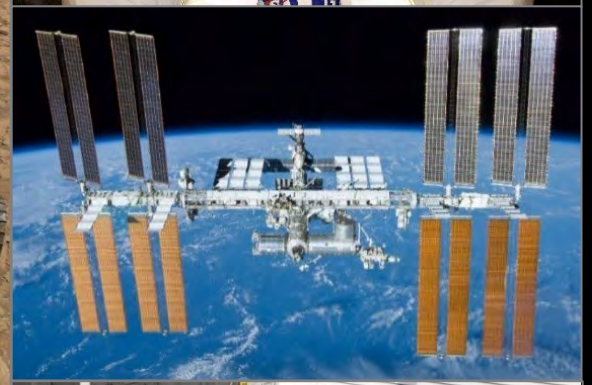


COURSE OVERVIEW

Module 1: Fundamental Concepts	Section 1: Introduction to Lithium-ion Batteries Section 2: Heat Generation from Electrochemical Processes	20 Minutes
Module 2: Battery Safety	Section 1: Defining Thermal Runaway Section 2: Safe Handling Practices Section 3: Abuse Testing Techniques Section 4: Addressing the Variance of Thermal Runaway Section 5: NASA's Response to Thermal Runaway Section 6: Safe Battery Design Related Lessons Learned	90 Minutes
Module 3: Modeling Techniques	Section 1: Practical Thermal Model Construction Techniques Section 2: Example Thermal Simulations Part 1, Nominal Operations Section 3: Example Thermal Simulations Part 2, Thermal Runaway	30 Minutes
	Wrap-Up and Questions Acknowledgements	10 Minutes



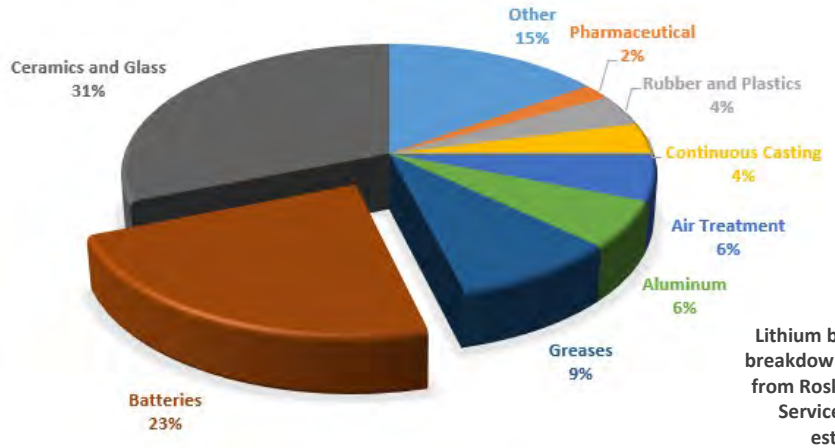



MODULE 1 SECTION 1: INTRODUCTION TO LITHIUM-ION BATTERIES

GLOBAL DEMAND FOR LITHIUM-ION BATTERIES

- **Lithium ion (Li-ion) batteries provide energy dense and low mass energy storage solutions for a wide array of applications including automobile, aerospace, industrial, medical, military, small portable electronics, railway, and space exploration:**
  - Growing demand for advanced energy storage systems drives the Li-ion battery market which is expected to reach $43 billion USD by 2020 [1, 11-13]



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


10


4


2


5


6


7


8



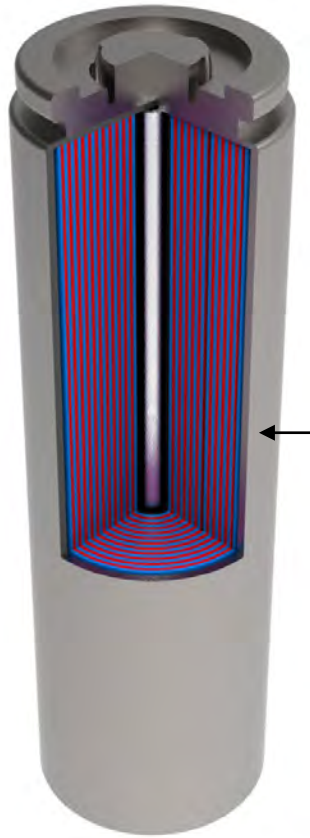
9


3

1 Energy and Capital, "Energy storage companies: investing in lithium batteries," 2012. [Online]. Available: https://www.energyandcapital.com/resources/energy-storage-companies.
2 Apple, "Why Lithium-ion?," Apple, [Online]. Available: https://www.apple.com/batteries/why-lithium-ion/. [Accessed 5 June 2015].
3 Tesla Motors, "Tesla Motors," Tesla Motors, [Online]. Available: http://www.teslamotors.com/en_GB/support. [Accessed 5 June 2015].
4 Milwaukee, "M18 Cordless 1/2" Hammer Drill/Driver (Bare Tool)," Milwaukee, [Online]. Available: http://www.milwaukeetool.com/power-tools/cordless/2602-20. [Accessed 5 June 2015].
5 Varta, "Li-ion battery cell / energy storage / flat CP series," Varta, [Online]. Available: http://www.directindustry.com/prod/varta-microbattery-gmbh/product-88149-1349927.html. [Accessed 15 June 2015].
6 C. Macmanus, "New Sony Rechargeable battery has 4x the lifespan of current lithium ion batteries," Sony, [Online]. Available: http://www.sonyinsider.com/2009/08/11/new-sony-rechargeable-battery-has-4x-the-lifespan-of-current-lithium-ion-batteries/. [Accessed 5 June 2015].
7 All-Battery, "Li-polymer 3.7V 3000mAh (506090) Battery," All-Battery, [Online]. Available: http://www.all-battery.com/polymerli-ionbattery37v3000mah506090.aspx. [Accessed 5 June 2015].
8 "Tenergy Li-ion prismatic (103450) 3.7V 1800mAh rechargeable battery," Tenergy, [Online]. Available: http://www.tenergy.com/30052. [Accessed 1 July 2015].
9 Smart Battery, "12V 50Ah Lithium ion battery 5850," Smart Battery, [Online]. Available: http://www.lithiumion-batteries.com/products/product/12v-50ah-lithium-ion-battery.php. [Accessed 15 June 2015].
10 Huber, M., "It's a bird, it's a plane, it's... an uber?", https://www.bjtonline.com/business-jet-news/its-a-bird-its-a-plane-itsan-uber. [Accessed 13 August 2018].
11 A. Franco, Rechargeable lithium batteries: from fundamentals to applications, London: Woodhead Publishing, 2015.
12 EnerSys, "EnerSys power/full solutions investors presentation," 2014.
13 C. Carella, "Frost & Sullivan, global lithium-ion market to double despite recent issues," 21 February 2013. [Online]. Available: http://www.frost.com/prod/servlet/press-release.pag?docid=274194514.

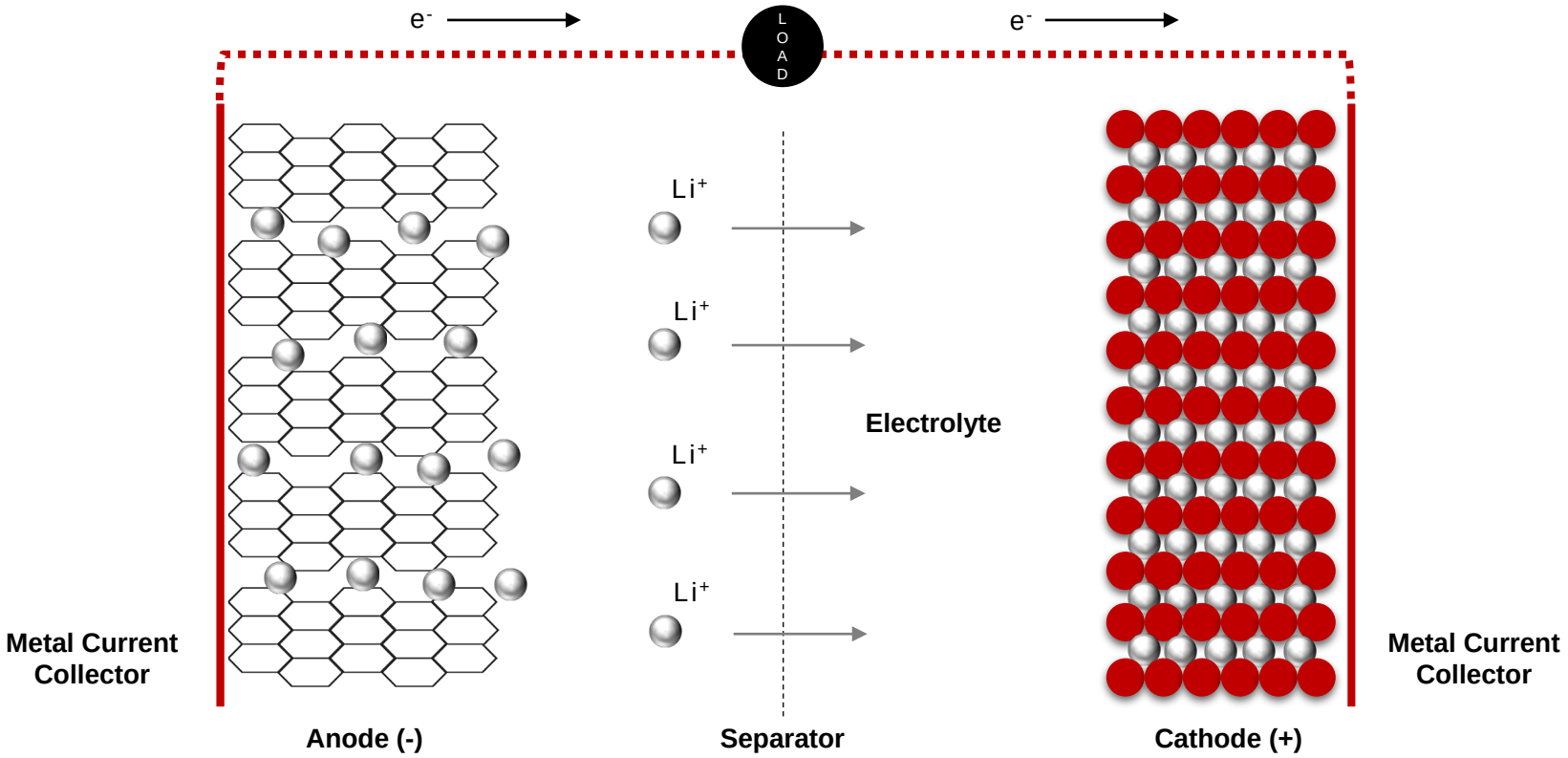
HOW LITHIUM-ION BATTERIES WORK

- **The primary components of Li-ion batteries are the anode, cathode, electrolyte and separator (collectively, this is the electrode winding or stack-up):**
  - 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 insulating separator to prevent internal short circuiting (i.e. the touching of electrodes)
  - Electrons flow through an external circuit
- **Li-ion batteries function with electrochemical reactions:**
  - Chemical reaction caused by or accompanied by an electrical current
  - Primary batteries: non-reversible reactions
  - Secondary batteries: reversible reduction-oxidation reactions occur at electrodes



Example image highlights the electrode winding of an 18650 cell

HOW LITHIUM-ION BATTERIES WORK



Schematic applies to discharge: reverse ion-electron flow for charge

HOW LITHIUM-ION BATTERIES WORK

- **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, $E = E^0 - \frac{RT}{nF} lnQ_R$
- **Example of half cell reactions, overall reaction, energy calculation and potential calculation provided (below) for the following electrode and electrolyte combination:**
  - Cathode (+): Lithium Cobalt Oxide ($LiCoO_2$)
  - Anode (-): Lithium graphite (LiC_6)
  - Electrolyte: Lithium hexafluorophosphate ($LiPF_6$)

Electrode Potential = $E^+ - E^-$ = 4 V

ΔG = -1 * 96500 C mol^{-1} * 4 V (i.e. 4 J C^{-1})

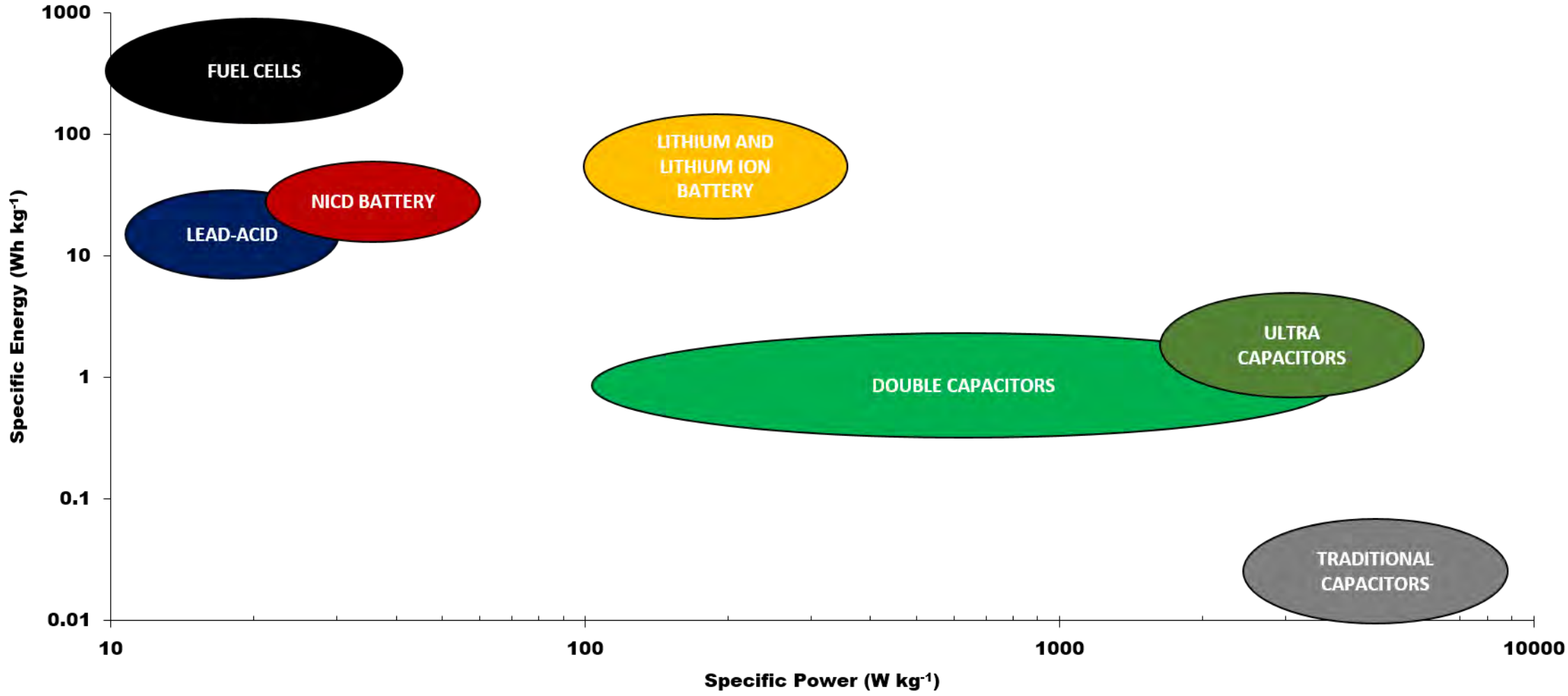
ΔG = -386 kJ = -107.2 Wh mol^{-1} @ 0.17 kg mol^{-1}

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

(+)	$CoO_2 + Li^+ + e^- \rightarrow LiCoO_2$	Reduction	E^0 = 1 V
(-)	$LiC_6 \rightarrow Li^+ + C6 + e^-$	Oxidation	E^0 = -3 V
Overall	$CoO_2 + LiC6 \rightarrow LiCoO_2 + C6$		n = 1

Discharge

RAGONE PLOT COMPARISON



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

DISADVANTAGES OF LITHIUM-ION BATTERIES

- **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 [15-16]
- **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)

15 Zhang, H., & Braun, P. V. (2012). Three-Dimensional Metal Scaffold Supported Bicontinuous Silicon Battery Anodes. *Nano Letters* , *12*, 2778-2783.
16 NASA Ares Laboratories, "Scanning Electron Microscopes Laboratory," NASA ARES, [Online]. Available: http://ares.jsc.nasa.gov/Laboratories/kr_laboratories/SEM.cfm. [Accessed 15 July 2015].

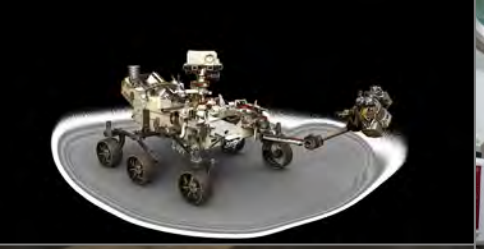
KEY TERMINOLOGY

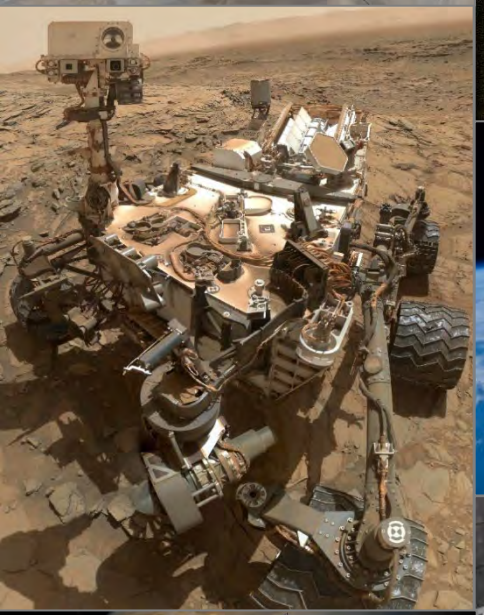
- **Cell** refers to a single Li-ion cell electrode winding
- **Battery** can refer to an assembly of Li-ion cells or can also refer to a single Li-ion cell (this is not common)
- **Banks**, **packs, and assemblies** refer to small assemblies of multiple cells; assemblies can also refer to an arrangement of multiple banks and packs
- **Open circuit voltage (OCV)** refers to the voltage difference between the electrode terminals when no current is applied; OCV is state-of-charge dependent
- **Working voltage (WV)** refers to the actual voltage during charge and discharge
- **Nominal voltage** is a mid-point voltage (or average voltage) representative of the overall voltage to expect between a battery being completely charged and completely discharged; the average voltage during charging is also referred to as nominal voltage
- **State-of-charge (SOC)** refers to the percent state of charge that the battery is at for any given point in time
- **Depth-of-discharge (DOD)** refers to how deeply the battery is discharged (also described in percent)
- **Jellyroll** or **electrode winding** are common terms used to describe the lay-up of cathode, anode, separator, and electrolyte
- **Cell casing** refers to the encapsulation material used to encase the electrode winding (e.g. the steel can for cylindrical cells)

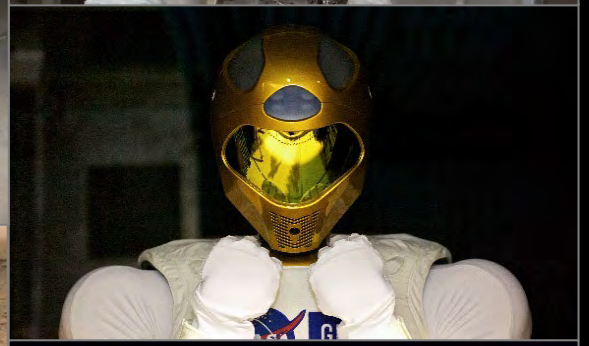
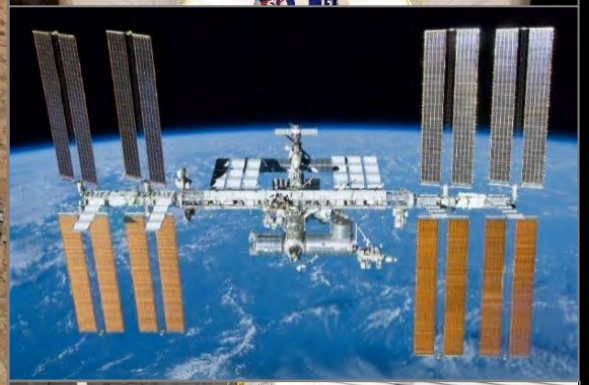
KEY TERMINOLOGY

- **Capacity** defines how much energy the cell can store and is typically rated based on 1-Coulomb, or 1-C (i.e. how many Amps can be pulled from the cell constantly for 1 hour when starting at 100% state-of-charge); e.g. a 1 Ah cell can provide 1 A for 1 hour

- **Coulomb** refers to the rate of charge or discharge in relationship to how quickly or slowly a full charge is reached (on charging) or a full charge is depleted (on discharge) – example for a 1 Ah cell provided below:
  - 0.2 C-rate (or C/5) allows 0.2 A to be drawn for 5 hours
  - 0.5 C-rate (or C/2) allows 0.5 A to be drawn for 2 hours
  - 1 C-rate allows 1 A to be drawn for 1 hour
  - 2 C-rate allows 2 A to be drawn for 0.5 hour (30 minutes)
  - 5 C-rate allows 5 A to be drawn for 0.2 hour (12 minutes)






MODULE 1 SECTION 2:

HEAT GENERATION FROM ELECTROCHEMICAL PROCESSES

HEAT GENERATION FROM ELECTROCHEMICAL PROCESSES

- **Sherfey and Brenner (1958) first identified that Li-ion battery electrochemical processes (i.e. charge and discharge) generate heat due to the over-potential and entropic reactions [17-20]:**
  - Over-potential refers to the difference between the open circuit voltage (V_{OC}) and the working voltage (V_W)
  - The over-potential exists due to chemical irreversibilities such as Ohmic losses (i.e. Joule heating from the movement of charged particles), charge-transfer over-potentials, and mass transfer limitations
  - Ohmic losses (or Joule heating) are a function of the resistance to particle travel between the electrodes
  - Entropic reactions refer to exothermic and endothermic reactions occurring inside the cell due to the transfer of ions and electrons
- **Bernardi et. al. (1985) developed an energy balance that expanded from the Sherfey and Brenner definition to represent the local heat generated in a Li-ion cell as a function of the following [17-20]:**
  - Voltage and current
  - Enthalpy of reaction (enthalpy voltage of reaction) and enthalpy of mixing
  - Phase change
  - Heat capacity change
- **For practical simulation purposes, the energy balance derived by Bernardi et. al. is commonly reverted to the original form presented by Sherfey and Brenner to only include the heat generation rates due to electrical work and entropy change:**

$$\mathbf{Q_{Cell} = I\left(\underbrace{V_{OC} - V_W}_{\text{Over-potential}} - \underbrace{T\frac{\partial V_{OC}}{\partial T}}_{\text{Entropic Heat}}\right)}$$

Q_{Cell}	Heat	W
I	Current	A
V_{OC}	Open Circuit Voltage	V
V_W	Working Voltage	V
T	Temperature	°C

17 J. M. Sherfey and A. Brenner, "Electrochemical Calorimetry," Journal of the Electrochemical Society, vol. 105, no. 11, 1958.
18 D. Bernardi, E. Pawlikowski and J. Newman, "A General Energy Balance for Battery Systems," Journal of the Electrochemical Society, vol. 132, no. 4, 1985.
19 T. Bandhauer et. al., "A critical review of thermal issues in lithium-ion batteries," Journal of the Electrochemical Society, vol. 158, no. 3, 2011
20 M. Keyser et. al., "Battery Thermal Characterization," NREL Report, 2015.

HEAT GENERATION FROM ELECTROCHEMICAL PROCESSES

- **Consumers of Li-ion battery technology should understand that both performance and safety are both temperature dependent:**
  - From a performance perspective, V_{OC}, V_W, and the entropy term from the Bernardi et. al. equation are all temperature dependent
  - Also from a performance perspective, operating the cells beyond the certified temperature ranges can permanently damage the cell
  - From a safety perspective, over-heating is one abuse type that can lead to thermal runaway (more discussion on this in Module 2)
  - Therefore, design consideration must be given to any mechanism that can change the internal temperature of the Li-ion battery
- **More thoughts from this instructor:**
  - From an analysis perspective, some analysts simplify nominal internal heat generation to be a function of the current multiplied by the internal resistance of the cell, which, per Ohm's law, also yields the heat generated from operating the cell
  - Unfortunately, this method yields a constant value, and as shown on the next few slides, will fail to adequately characterize the thermal profile of a given cell during charge and discharge operations – including peak temperatures
  - This instructor recommends always considering the effects of temperature and voltage change on charge and discharge heat generation rates

EXAMPLE OF HEAT GENERATION FROM ELECTROCHEMICAL PROCESSES FOR DISCHARGE

- **Discharge example for a large format 185 Ah $LiCoO_2$ electric vehicle battery based on Chen et. al. [19] and Walker et. al. [20] which compared test and analysis for various discharge rates and convective cooling environment combinations**

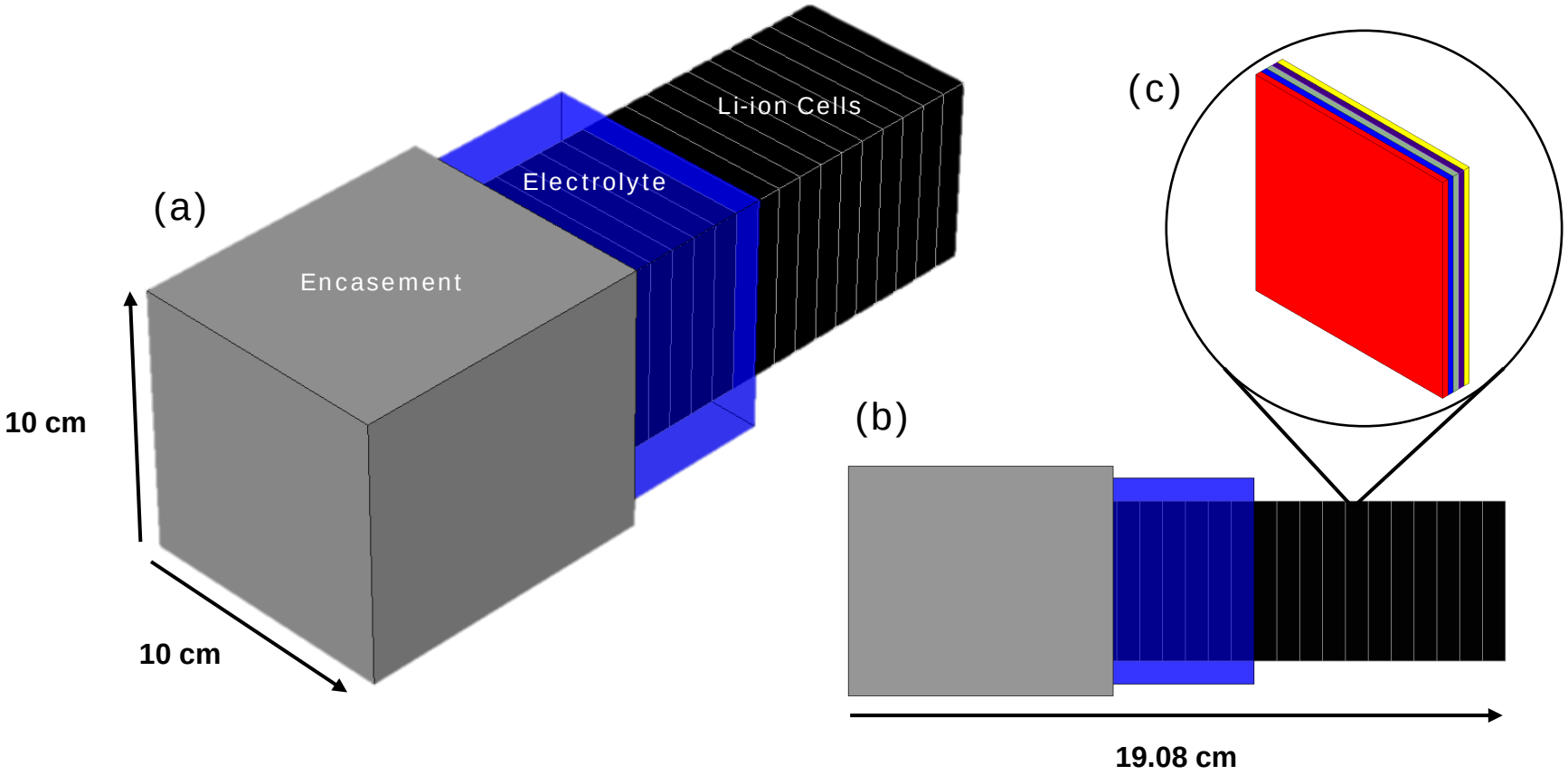


Image courtesy of Walker and Ardebili [20]

19 S. Chen, C. Wan and Y. Wang, "Thermal Analysis of Lithium-Ion Batteries," Journal of Power Sources, vol. 140, pp. 111-124, September 2005.
20 W. Walker and H. Ardebili, "Thermo-electrochemical analysis of lithium ion batteries for space applications using Thermal Desktop," Journal of Power Sources, vol. 269, pp. 486-497, 2014.

EXAMPLE OF HEAT GENERATION FROM ELECTROCHEMICAL PROCESSES FOR DISCHARGE

- **Discharge example for a large format 185 Ah $LiCoO_2$ electric vehicle battery based on Chen et. al. [19] and Walker et. al. [20] which compared test and analysis for various discharge rates and convective cooling environment combinations**

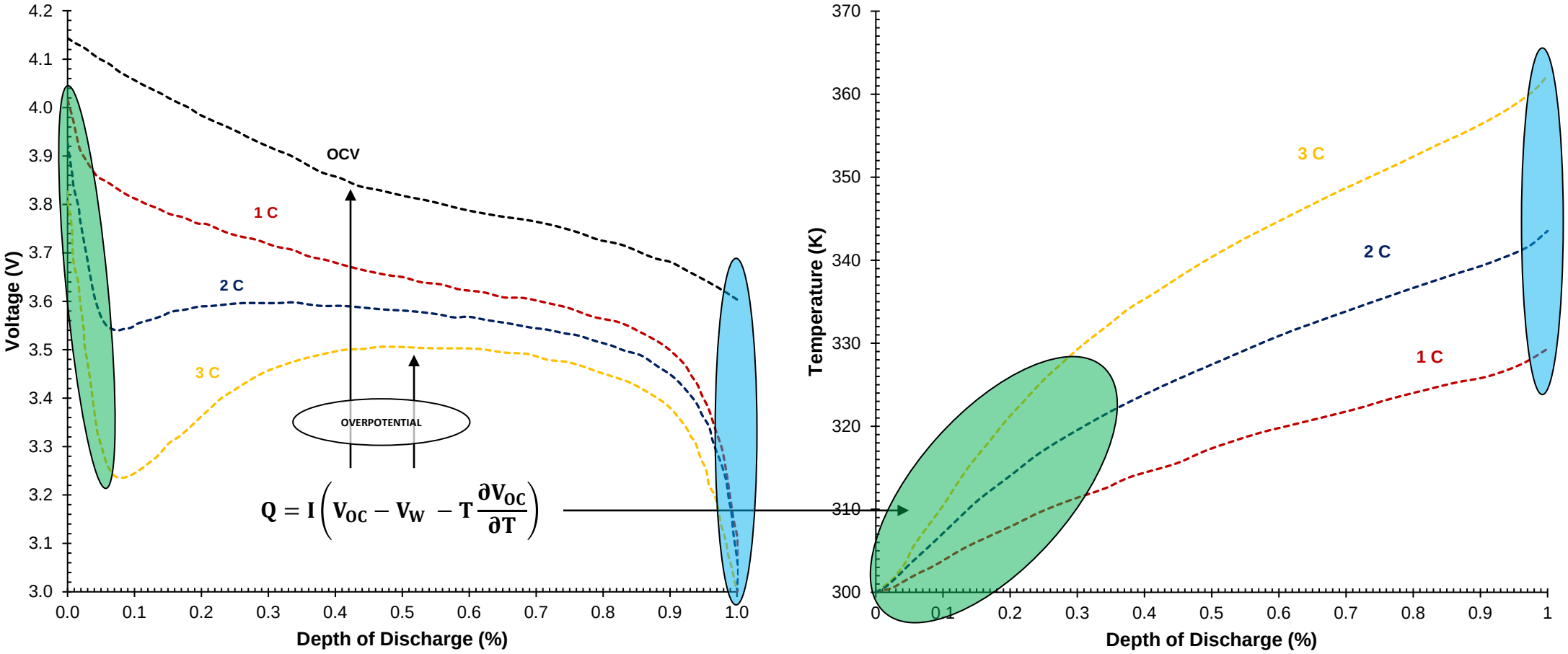


Image courtesy of Walker and Ardebili [20]

19 S. Chen, C. Wan and Y. Wang, "Thermal Analysis of Lithium-Ion Batteries," Journal of Power Sources, vol. 140, pp. 111-124, September 2005.
20 W. Walker and H. Ardebili, "Thermo-electrochemical analysis of lithium ion batteries for space applications using Thermal Desktop," Journal of Power Sources, vol. 269, pp. 486-497, 2014.

EXAMPLE OF HEAT GENERATION FROM ELECTROCHEMICAL PROCESSES FOR CHARGE

- **Charge example based on various charging rates of a Boston Power Swing 5300 Li-ion cell [21] and Walker et. al. [22] :**
  - Note that this example does not employee constant current like the discharge example (see current profile on bottom left image)

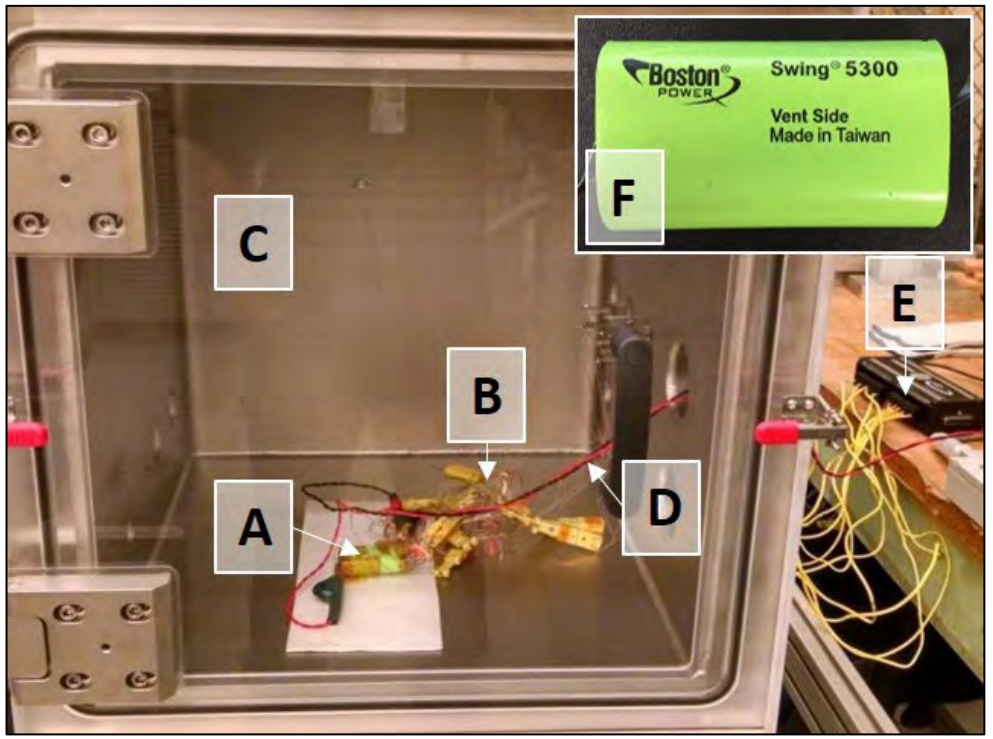


Image courtesy of Walker et. al. [22]

21 Boston Power, *Swing 5300 Rechargeable Lithium-ion Cell*, Westborough: Boston-Power, Incorporated, 2013.
22 W. Walker, S. Yayathi, J. Shaw and H. Ardebili, "Thermo-electrochemical evaluation of lithium-ion batteries for space applications." Submitted to Journal of Power Sources June 27th, 2015.

EXAMPLE OF HEAT GENERATION FROM ELECTROCHEMICAL PROCESSES FOR CHARGE

- **Charge example based on various charging rates of a Boston Power Swing 5300 Li-ion cell [21] and Walker et. al. [22]:**
  - Note that this example does not employee constant current like the discharge example (see current profile on bottom left image)

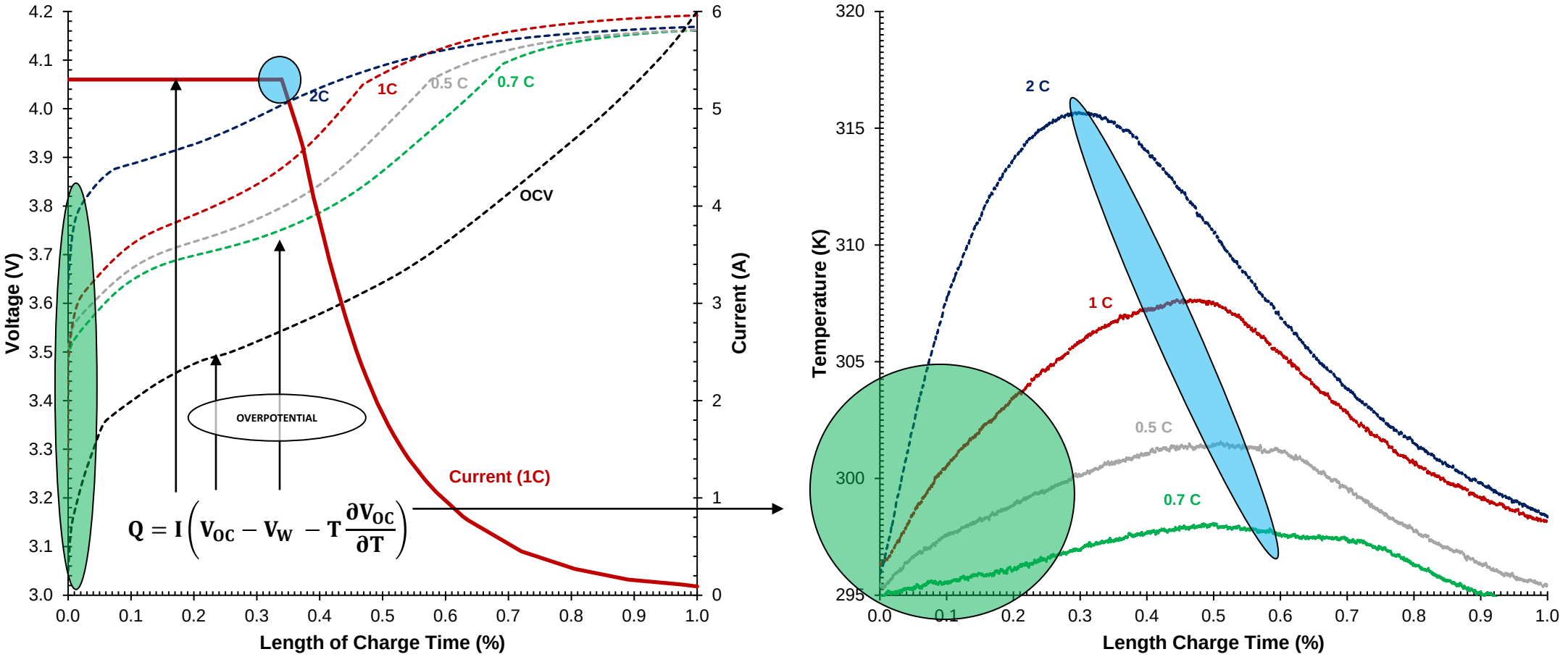


Image courtesy of Walker et. al. [22]

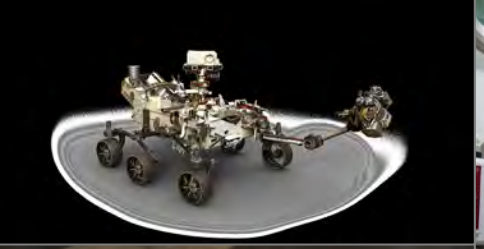
21 Boston Power, *Swing 5300 Rechargeable Lithium-ion Cell*, Westborough: Boston-Power, Incorporated, 2013.
22 W. Walker, S. Yayathi, J. Shaw and H. Ardebili, "Thermo-electrochemical evaluation of lithium-ion batteries for space applications." Submitted to Journal of Power Sources June 27th, 2015.

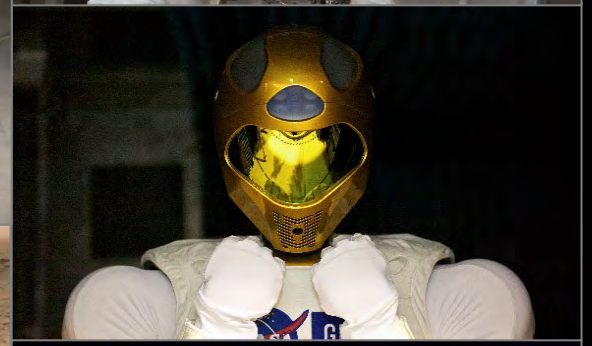
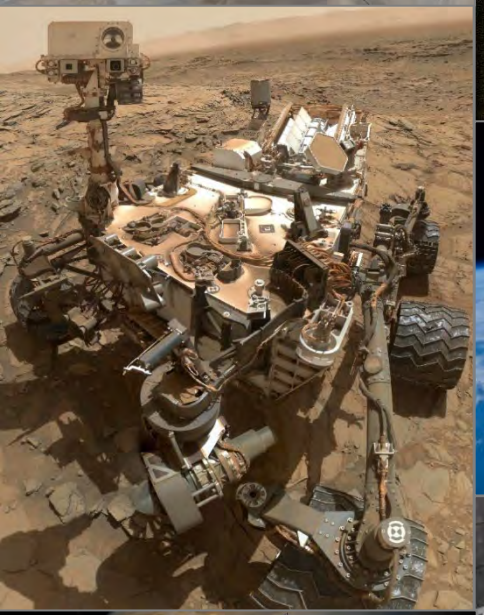
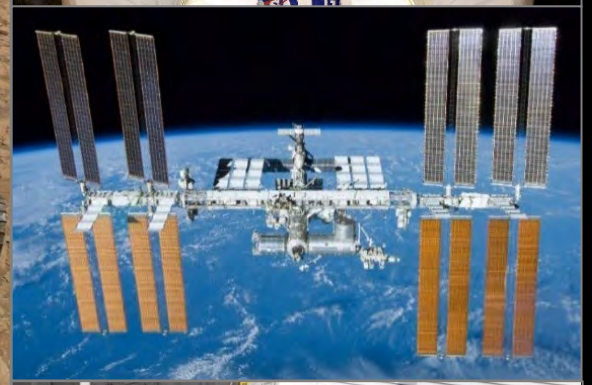
TEMPERATURE DEPENDENCE OF HEAT GENERATION RATES

- **The previous two examples were for charge and discharge at room temperature (i.e. one set of voltage profiles)**
- **For analysis purposes, this instructor recommends considering this problem with bi-variate arrays to take into account the temperature dependencies of working voltage and open circuit voltage:**
  - Bi-variate arrays can be populated with manufacturer data commonly provided in datasheets or can easily be developed with cycle testing
  - More on coupling this technique with the Bernardi et. al. energy balance for analysis is provided in Module 3

Can be time, state-of-charge, or depth-of-discharge depending on the analysis

	-45°C	-25°C	0°C	+25°C	+45°C
0min	#	#	#	#	#
10min	#	#	#	#	#
20min	#	#	#	#	#
30min	#	#	#	#	#
40min	#	#	#	#	#
50min	#	#	#	#	#
60min	#	#	#	#	#
70min	#	#	#	#	#





MODULE 2 SECTION 1:
DEFINING THERMAL RUNAWAY

DEFINING THERMAL RUNAWAY

- **Safety concerns exist for lithium-ion (Li-ion) battery utilization due to the inherent possibility of thermal runaway (TR)**
- **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
  - 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
- **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**

THERMAL RUNAWAY KINETIC RELATIONSHIPS

Richard and Dahn (1999) [23]

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

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

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

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

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

Heating due to SEI and anode decomposition

Hatchard et. al. (2001) [24]

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

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

Heating due to cathode decomposition

Kim et. al. (2007) [25]

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

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

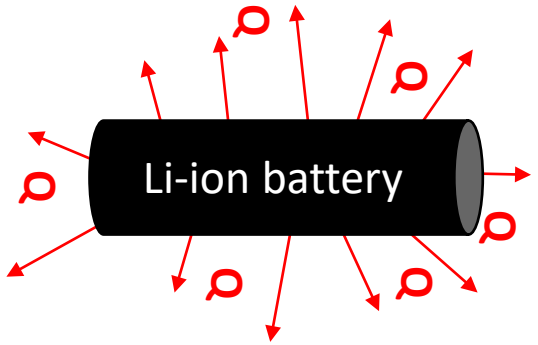
Heating due to electrolyte decomposition

Coman et. al. (2015) [26]

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

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

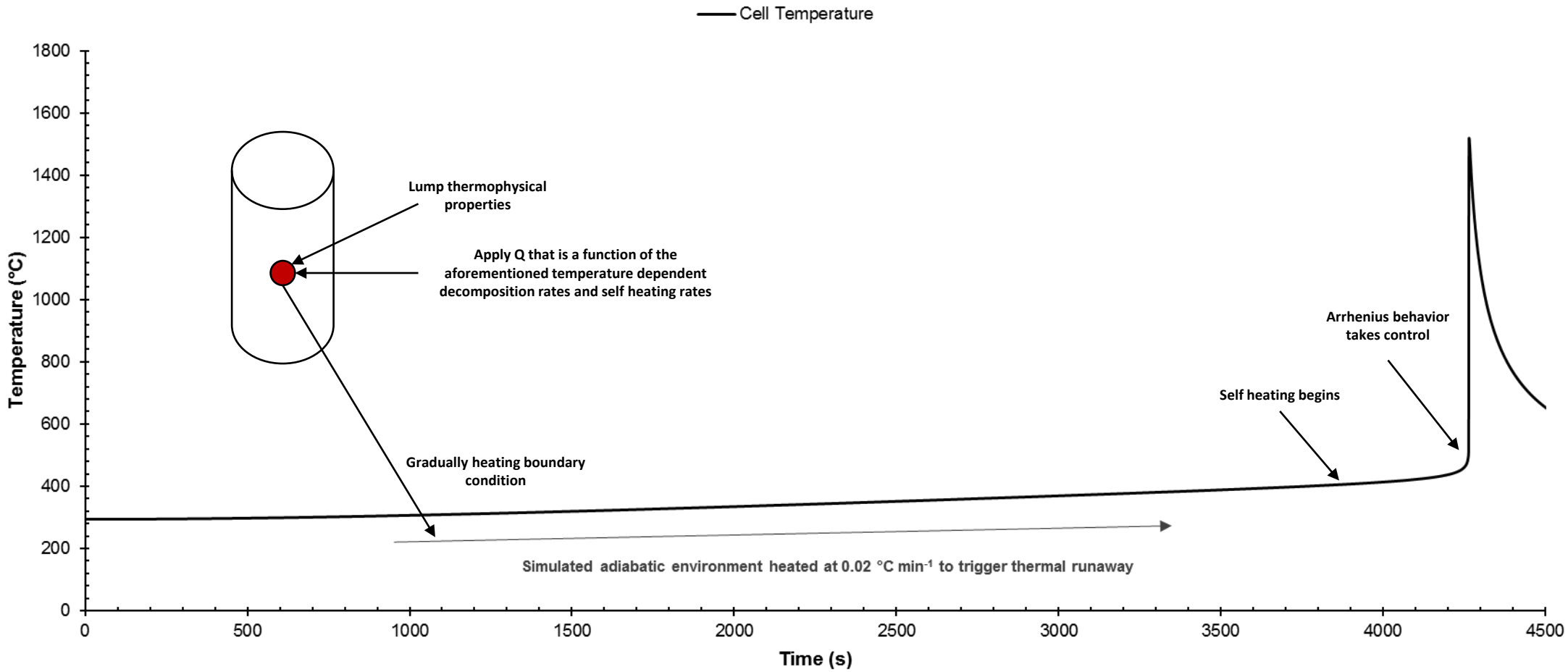
Heating due release of electrochemical energy



A	Frequency Factor
x, Y	Fraction
E	Activation Energy
k_b	Boltzmann Constant
T	Temperature
z	Tunneling Term
m	Mass
h	Enthalpy
t	Time
Q	Heat
SOC	State-of-Charge

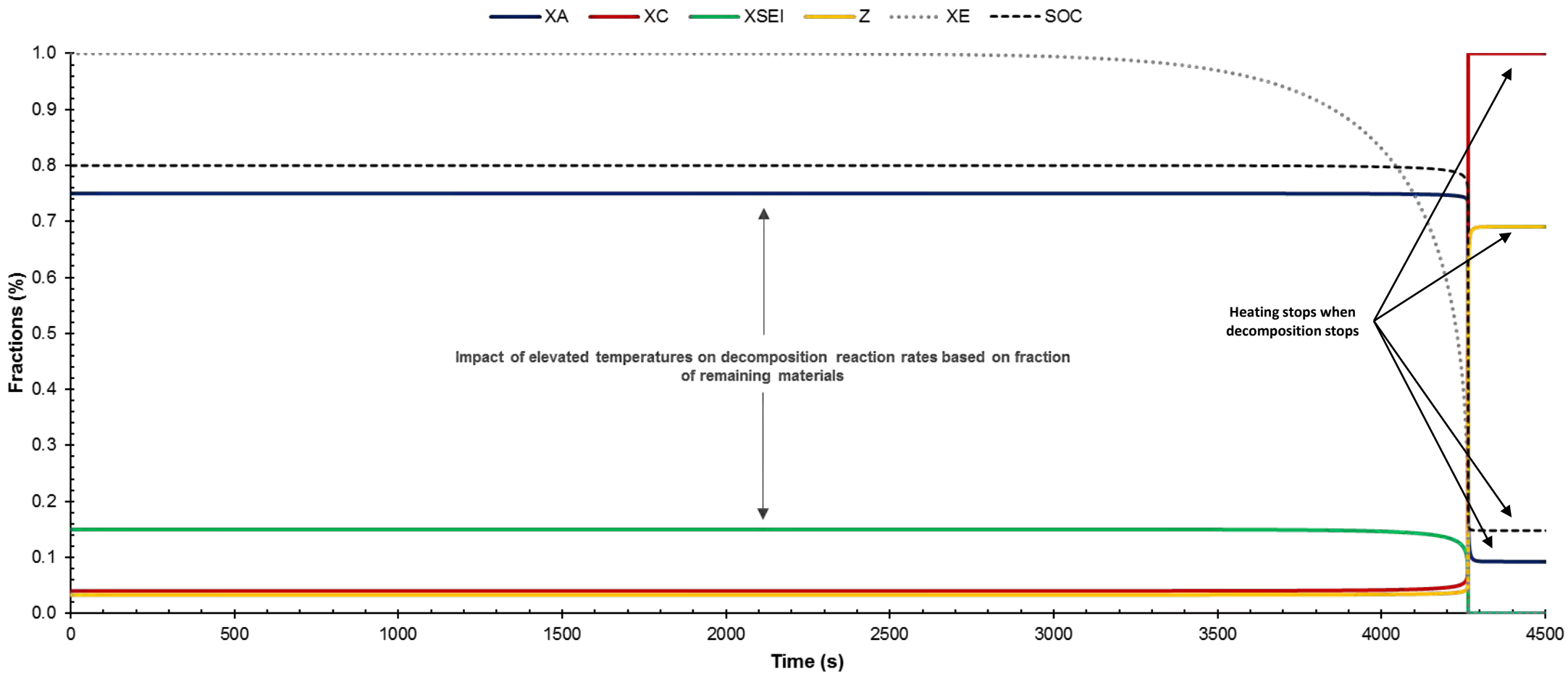
23 Richard, M. Accelerating rate calorimetry study on the thermal stability of lithium intercalated graphite in electrolyte. I. experimental. *Journal of The Electrochemical Society* **146,** 2068 (1999).
24 Hatchard, T., MacNeil, D., Basu, A. & Dahn, J. Thermal model of cylindrical and prismatic lithium-ion cells. *Journal of The Electrochemical Society* **148,** A755 (2001).
25 Kim, G.-H., Pesaran, A. & Spotnitz, R. A three-dimensional thermal abuse model for lithium-ion cells. *Journal of Power Sources* **170,** 476–489 (2007).
26 Coman, P., Rayman, S. & White, R. A lumped model of venting during thermal runaway in a cylindrical Lithium Cobalt Oxide lithium-ion cell. *J Power Sources* **307,** 56–62 (2016).

THERMAL RUNAWAY KINETIC RELATIONSHIPS (0-D EXAMPLE)



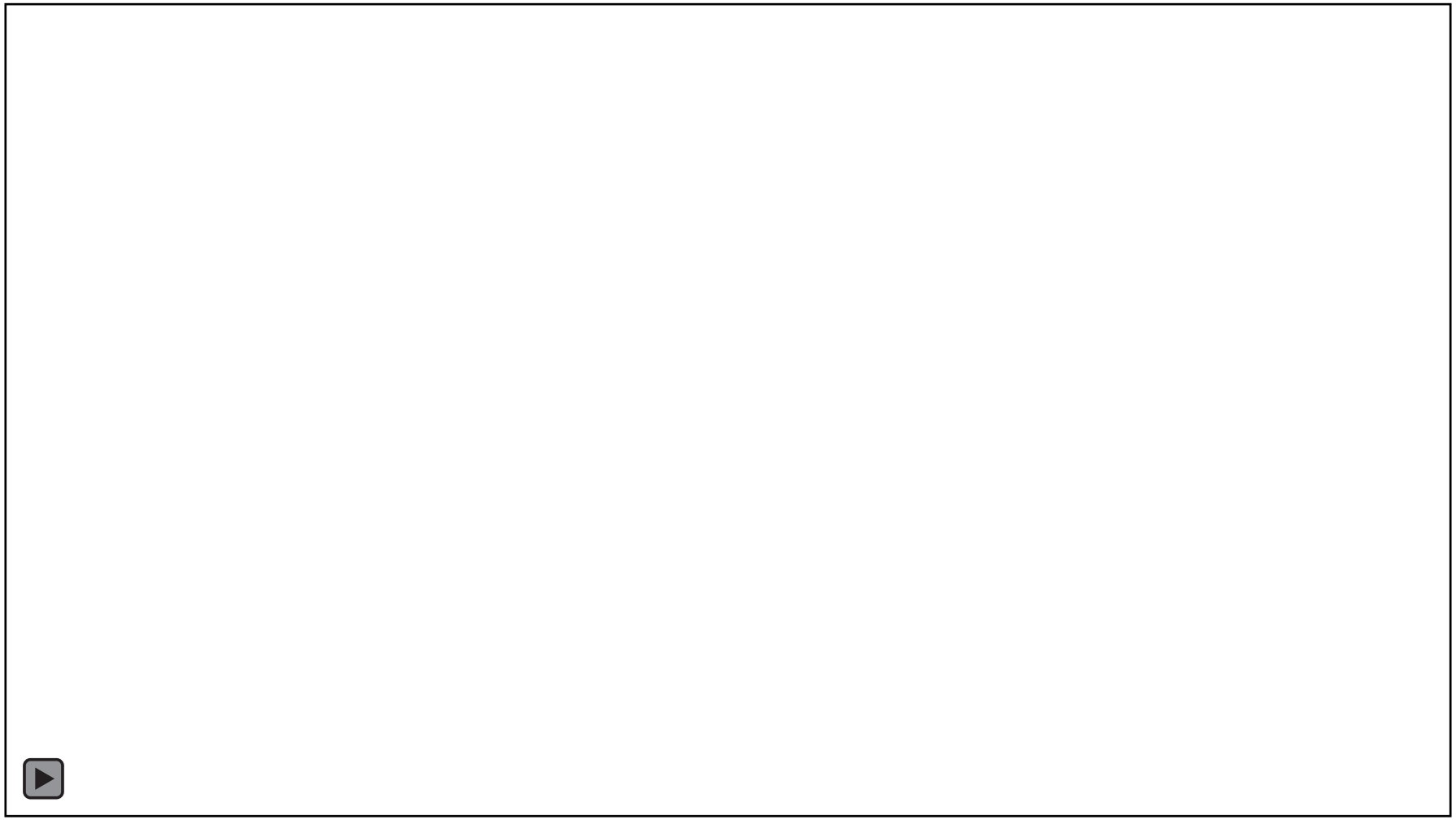
23 Richard, M. Accelerating rate calorimetry study on the thermal stability of lithium intercalated graphite in electrolyte. I. experimental. *Journal of The Electrochemical Society* **146,** 2068 (1999).
24 Hatchard, T., MacNeil, D., Basu, A. & Dahn, J. Thermal model of cylindrical and prismatic lithium-ion cells. *Journal of The Electrochemical Society* **148,** A755 (2001).
25 Kim, G.-H., Pesaran, A. & Spotnitz, R. A three-dimensional thermal abuse model for lithium-ion cells. *Journal of Power Sources* **170,** 476–489 (2007).
26 Coman, P., Rayman, S. & White, R. A lumped model of venting during thermal runaway in a cylindrical Lithium Cobalt Oxide lithium-ion cell. *J Power Sources* **307,** 56–62 (2016).

THERMAL RUNAWAY KINETIC RELATIONSHIPS (0-D EXAMPLE)



23 Richard, M. Accelerating rate calorimetry study on the thermal stability of lithium intercalated graphite in electrolyte. I. experimental. *Journal of The Electrochemical Society* **146,** 2068 (1999).
24 Hatchard, T., MacNeil, D., Basu, A. & Dahn, J. Thermal model of cylindrical and prismatic lithium-ion cells. *Journal of The Electrochemical Society* **148,** A755 (2001).
25 Kim, G.-H., Pesaran, A. & Spotnitz, R. A three-dimensional thermal abuse model for lithium-ion cells. *Journal of Power Sources* **170,** 476–489 (2007).
26 Coman, P., Rayman, S. & White, R. A lumped model of venting during thermal runaway in a cylindrical Lithium Cobalt Oxide lithium-ion cell. *J Power Sources* **307,** 56–62 (2016).

THERMAL RUNAWAY EXAMPLE



Video provided courtesy of Yayathi et. al. [31].

27 Yayathi, et. al., J. of Power Sources, 329 (2016) 197-206.

THERMAL RUNAWAY EXAMPLE

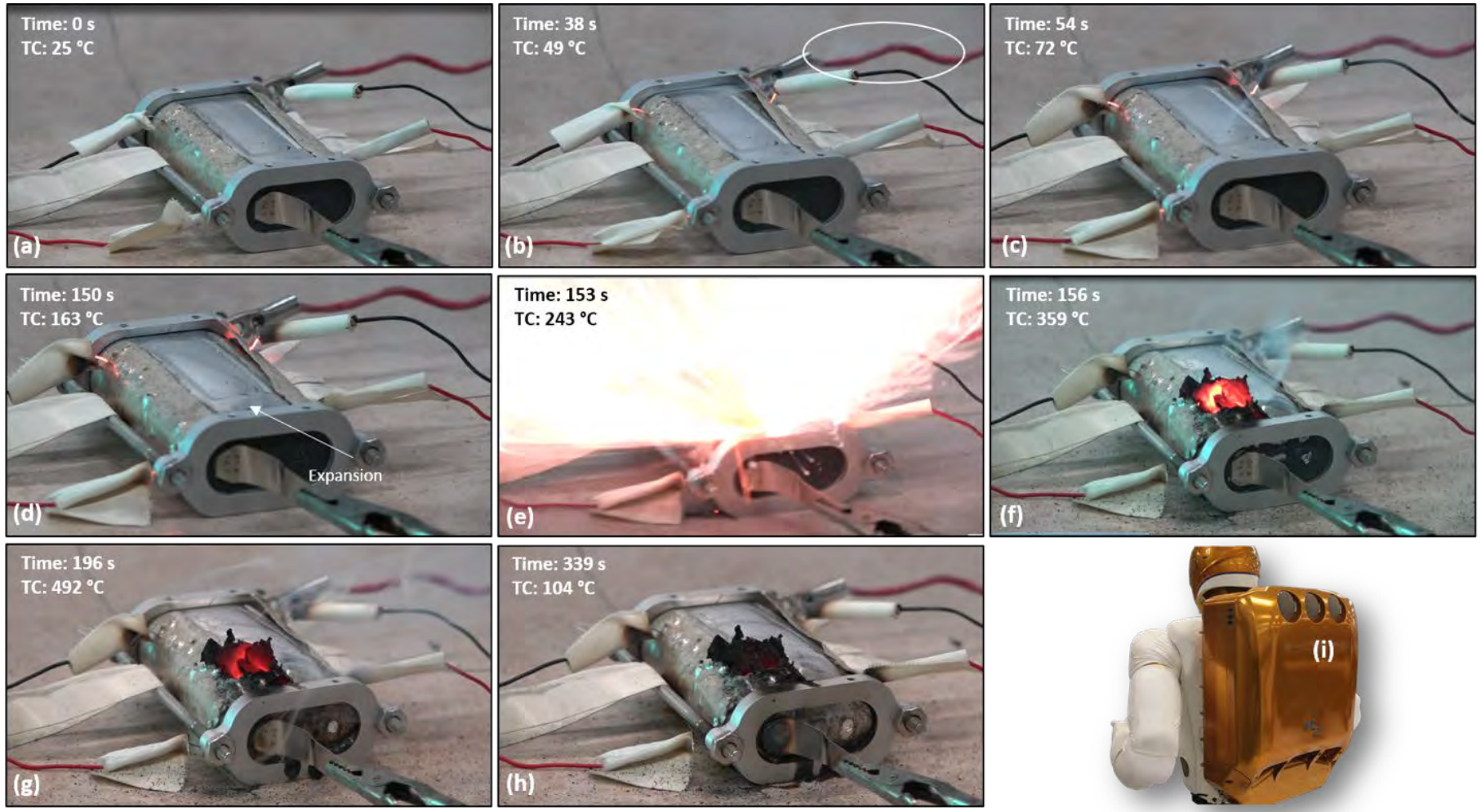


Image provided courtesy of Yayathi et. al. [31].

27 Yayathi, et. al., J. of Power Sources, 329 (2016) 197-206.

EXAMPLE FIELD FAILURES







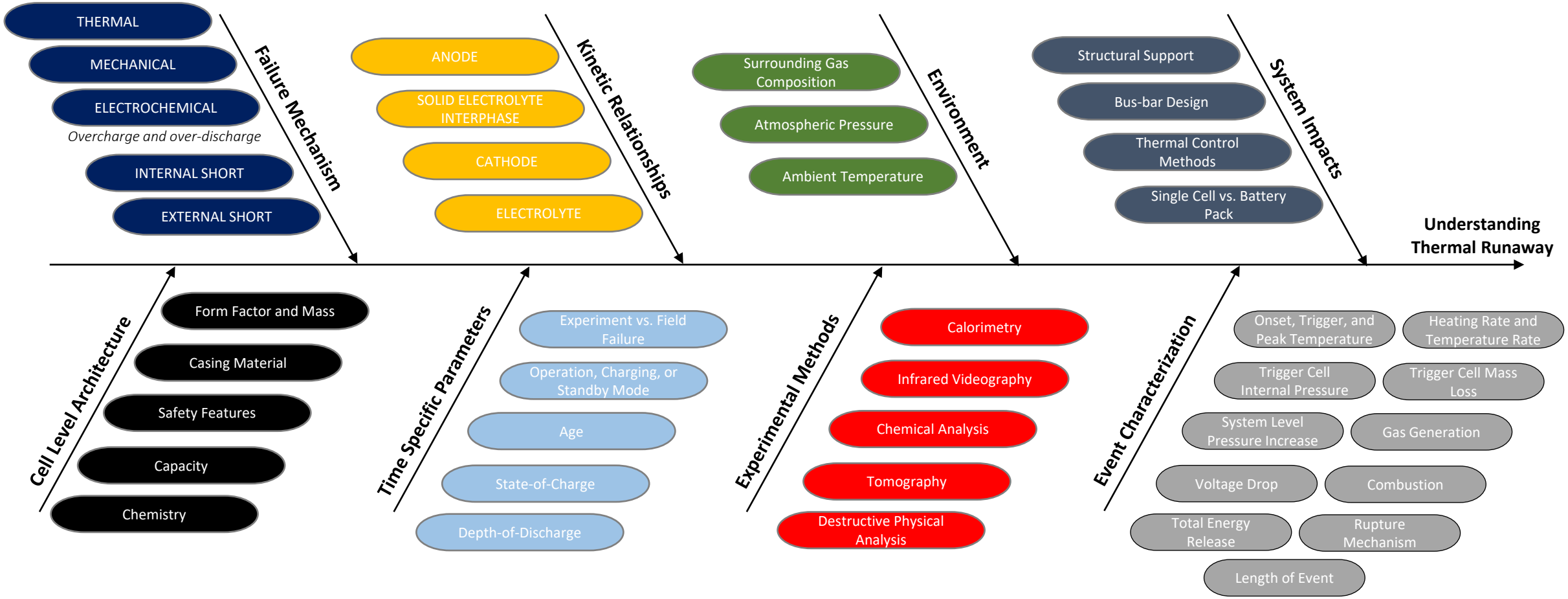


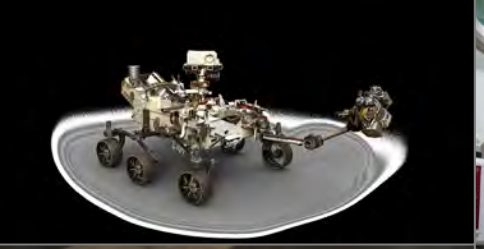


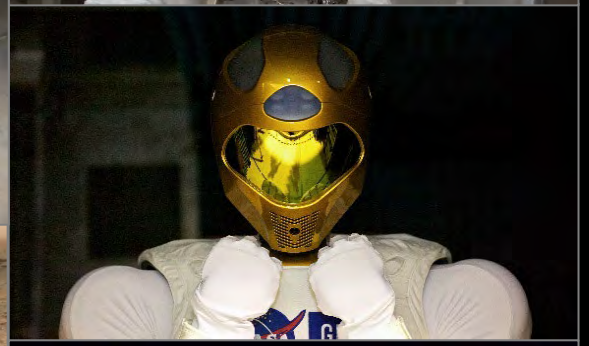
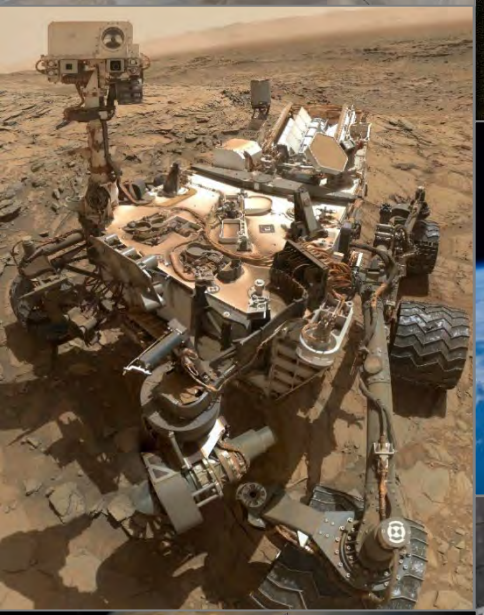
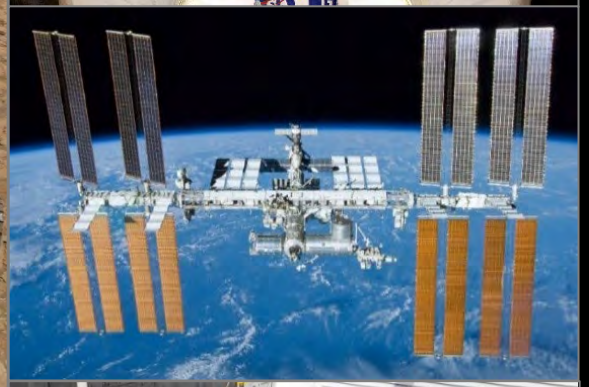


28 Gear Junkie. "Hoverboard image." [Online]. Available: https://gearjunkie.com/hoverboards-catch-fire-investigation
29 Airliners.Net, "Picture of the Boeing 747-44AF/SCD Aircraft," Airliners.Net, [Online]. Available: http://www2.airliners.net/photo/United-Parcel-Service/Boeing-747-44AF-SCD/1428553/L/. [Accessed 26 July 2015].
30 https://www.emirates247.com/news/emirates/lithium-batteries-linked-to-ups-air-crash-in-uae-us-2010-10-09-1.301382 [Accessed16 August 2018]
31 https://www.teslarati.com/tesla-model-s-burns-fire-supercharger-norway/
32 https://www.greenbot.com/article/3130453/android/report-samsung-is-still-struggling-to-explain-why-the-note7-keeps-exploding.html
33National Transportation Safety Board, 2014. *Interim Factual Report DCA13IA047,* Washington: NTSB.
34 Image courtesy of NASA

UNDERSTANDING THERMAL RUNAWAY

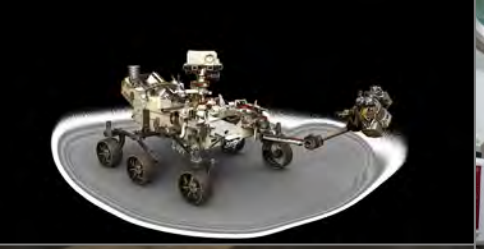


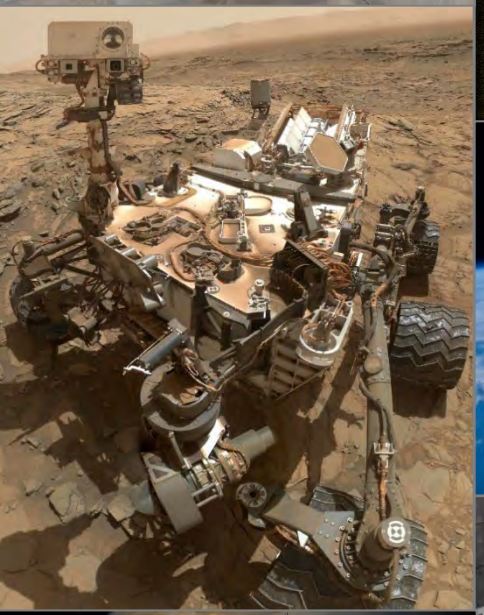


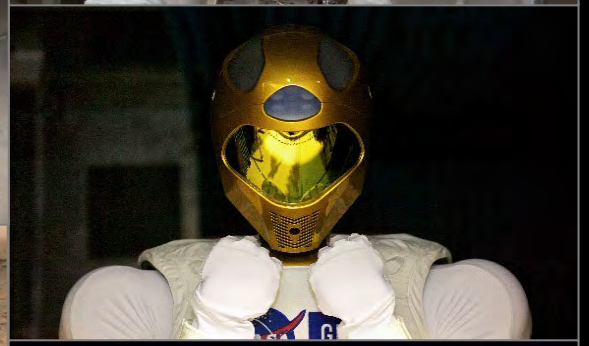
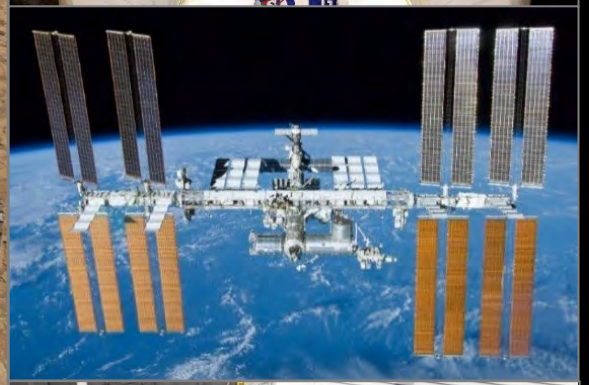







MODULE 2 SECTION 2:
SAFE HANDLING PRACTICES






MODULE 2 SECTION 3:
ABUSE TESTING TECHNIQUES

AVAILABLE CALORIMETRY METHODS

- **Thermal runaway is usually characterized with a variety of calorimetric methods**
- **Accelerating rate calorimetry (ARC) [31]:**
  - Very helpful in determining the onset temperature for TR and characterizing cell body heating rates
  - Due to the slow transient nature of the ARC test cycle, cell venting of the electrolyte occurs hours before TR
  - Early venting dries out the electrolyte
  - Dried electrolyte possibly degrades the total heat output
  - No practical means to discerning TR energy fractions
- **Bomb or steel can calorimetry [32, 33]:**
  - Adequate for determining total heat output
  - No practical means to discerning TR energy fractions
- **Copper slug calorimetry [34]:**
  - Effective for measuring the heat output through the cell casing
  - Does not measure the heat output through the ejecta
  - Estimates rate of mass ejected during TR
  - Must combine with bomb (steel can) calorimetry to calculate heat released through ejecta and gas
  - Again, no practical means to discern TR energy fractions

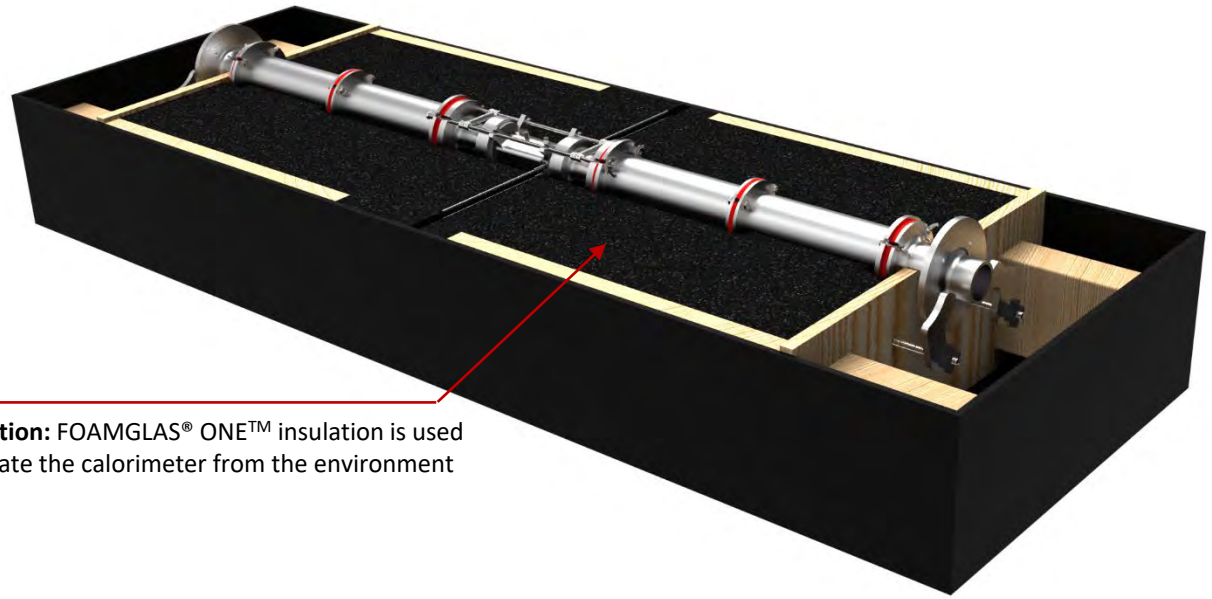


Image courtesy of Yayathi, et. al. [31]

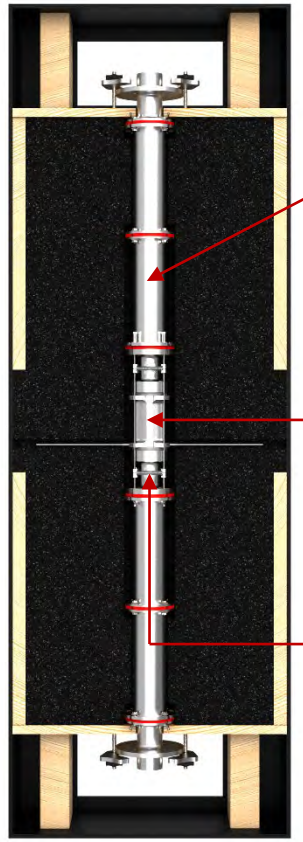
31 Yayathi, et. al., J. of Power Sources, 329 (2016) 197-206.
32 Walters, R.N. and Lyon R.E., Report DOT/FAA/TC-15/40, March 2016.
33 Jhu, C.Y., et. al., J. of Hazardous Materials, 192 (2011) 99-107.
34 Liu, X., et. al., J. of Power Sources, 280 (2015) 516-525.

FRACTIONAL THERMAL RUNAWAY CALORIMETRY

- **As an NESC assessment, NASA developed a new fractional TR calorimetry (FTRC) method for 18650-format Li-ion cells:**
  - Collaborators included NESC, NASA JSC, and SAIC
  - Allows discernment between (1) total heat output and (2) fraction of heat released through the cell casing vs. ejecta material
  - The energy distributions are determined by post processing temperature vs. time for each calorimeter sub-assembly (i.e. $\sum m_i C_{p_i} dT_i$)
  - Ambidextrous configuration accommodates cell designs with bottom vents (BVs)
  - Uses high flux heaters to initiate TR quickly (i.e. relevant to field failure)
  - Simple operation enables multiple experiments per day
  - Compatible with high speed X-ray videography [9]
  - Optional interface for measuring the gas exhaust heat



Insulation: FOAMGLAS® ONE™ insulation is used to isolate the calorimeter from the environment



Ejecta Bore Assemblies: Slow down and extract heat from escaping flames and gas

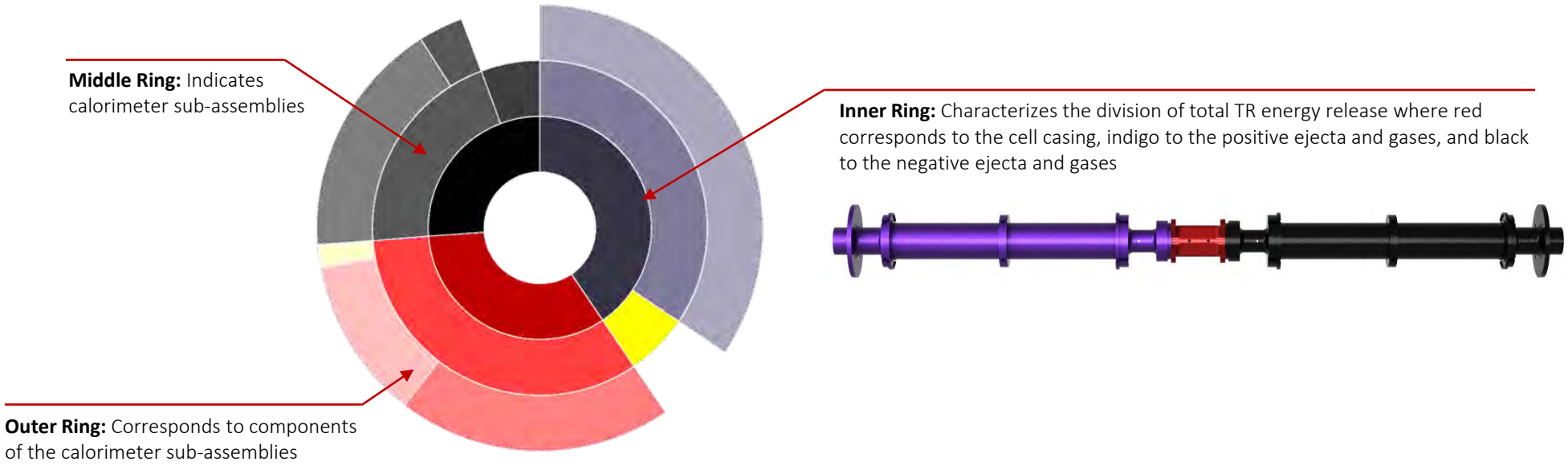
Cell Chamber Assembly: Includes heating system for thermally induced failure and mounting point for nail penetration system

Ejecta Mating Assemblies: Captures ejected solids such as the electrode winding

Images and data analysis submitted to J. Power Sources August 2018

FRACTIONAL THERMAL RUNAWAY CALORIMETRY

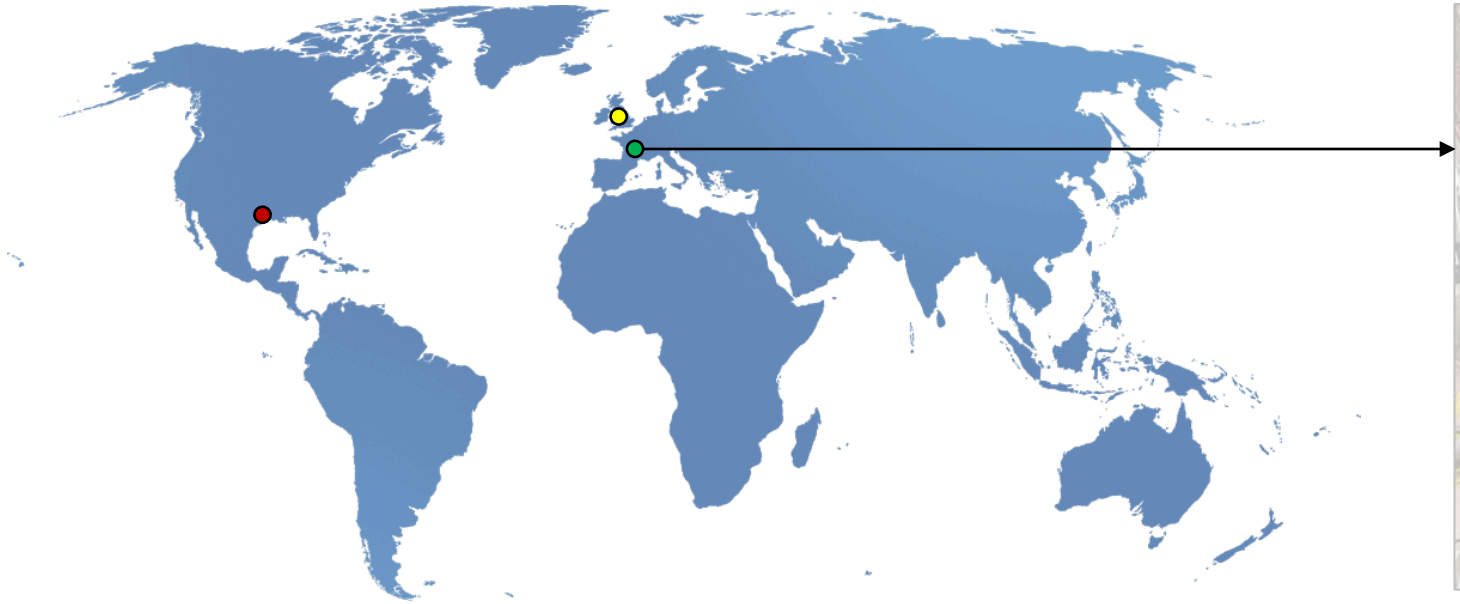
- **The calculated energy fractions are traceable to every calorimeter assembly, sub-assembly, and individual component**
- **The primary assemblies used for fractional calculations are the following:**
  - Cell Chamber Assembly (Red)
  - Positive Ejecta Mating Assembly (Indigo)
  - Positive Ejecta Bore Assembly (Indigo)
  - Negative Ejecta Mating Assembly (Black)
  - Negative Ejecta Bore Assembly (Black)



Images and data analysis submitted to J. Power Sources August 2018

FRACTIONAL THERMAL RUNAWAY CALORIMETRY

- **Images below depict the global testing capability of the device:**
  - FTRC testing at the NASA JSC Energy Systems Test Area (Red Dot)
  - FTRC testing at the European Synchrotron Radiation Facility (ESRF) for in-situ high speed tomography (Green Dot)
  - FTRC testing at the Diamond Light Source (DLS) Facility for in-situ high speed tomography (Yellow Dot)



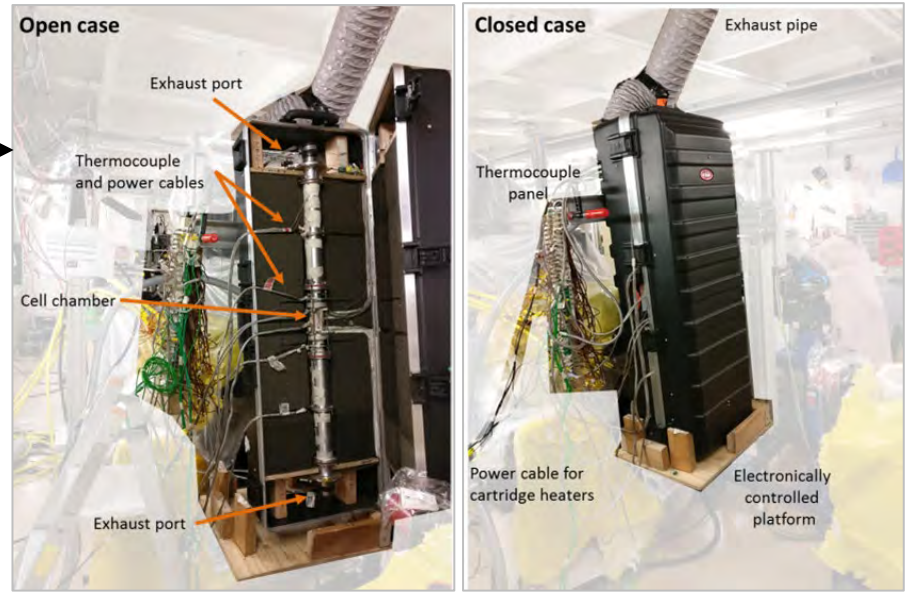
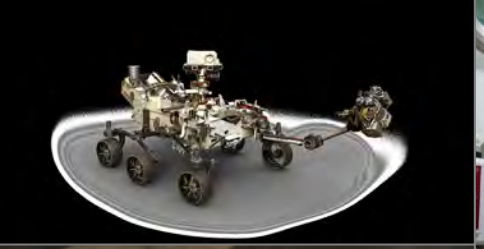


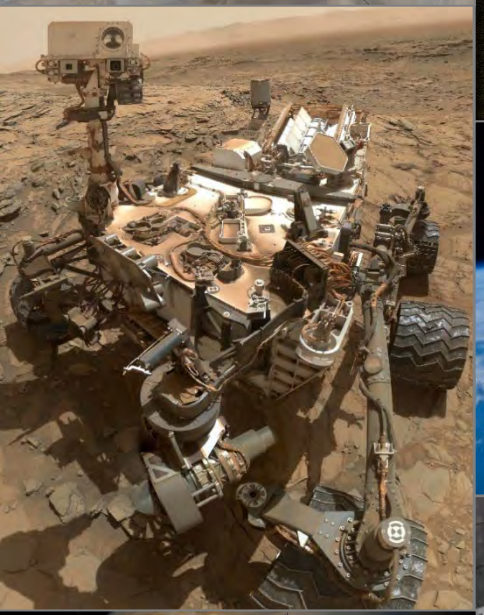
Image courtesy of Dr. Donal Finegan and ESRF

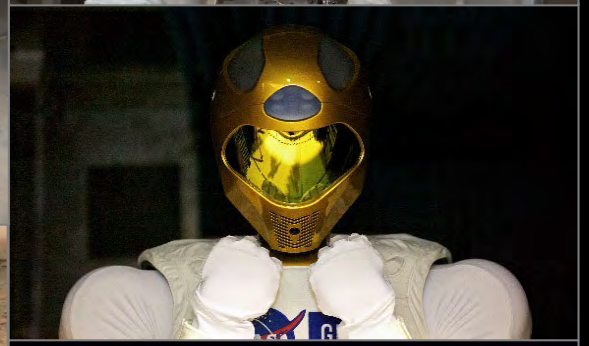
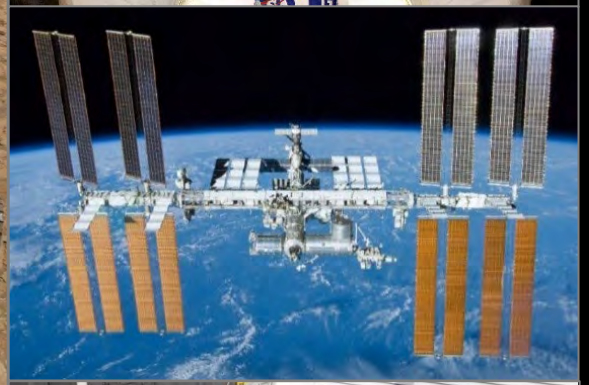
FRACTIONAL THERMAL RUNAWAY CALORIMETRY



Video courtesy of Dr. Donal Finegan (NREL) and ESRF






MODULE 2 SECTION 4:

ADDRESSING THE VARIANCE OF THERMAL RUNAWAY

DESCRIPTION OF CELL TYPES AND VARIABLES TESTED

- **The TR behavior of a variety of cell types, with varying chemistries and safety features, has been characterized:**
  - 3.35 Ah LG 18650 control groups consider the effects of bottom vent mechanisms (BV) vs. non-bottom vent (non-BV) mechanisms and the cell casing thickness (220 vs. 250 µm)
  - Molicel 18650-J control groups consider standard polymer separators and Dreamweaver gold and silver separators
  - Some of the 3.35 Ah LG 18650 cells and Molicel 18650-J cells had the NASA/NREL developed internal short circuiting (ISC) devices installed to examine TR behavior at lower temperatures (i.e. closer to field failure conditions); image below depicts the device
  - All cells were tested at 100% state of charge
- **Most experiments are conducted with high flux heaters for a trigger mechanism:**
  - For select cells, some of the FTRC experiments were conducted with nail penetration as well

Variable	Unit	LG18650-MJ1	3.35 Ah LG 18650	Cadenza 18650	Panasonic 18650-BE	Sony 18650-VC7	Samsung 18650-30Q	LG 18650-HE2	Molicel 18650-J
Capacity at 100% SOC	**Ah**	3.43	3.35	3.3	3.2	3.0	3.0	2.5	2.3
Nominal Voltage	**V**	3.67	3.7		3.6	3.6	3.6	3.6	3.78
Venting Mechanism	**-**	Non-BV	BV and Non-BV	Non-BV	BV	BV	Non-BV	Non-BV	Non-BV
Casing Thickness	**µm**	150	220 and 250		125		170		203
Internal Short Circuit [1]	**-**	No	Yes	No	No	No	No	No	Yes
Trigger Mechanism	**-**	Heat/Nail	Heat/Nail	Heat	Heat	Heat	Heat	Heat	Heat/Nail
Separator Material	**-**	-	-	-	-	-	-	-	Poly, Ag, Au
Count [2]	**-**	15	40	3	2	9	5	3	15

[1] The ISC device was only installed in some of the cells

[2] The count refers to the total number of cells tested per cell type

DESCRIPTION OF CELL TYPES AND VARIABLES TESTED

- **The TR behavior of a variety of cell types, with varying chemistries and safety features, has been characterized:**
  - 3.35 Ah LG 18650 control groups consider the effects of bottom vent mechanisms (BV) vs. non-bottom vent (non-BV) mechanisms and the cell casing thickness (220 vs. 250 µm)
  - Molicel 18650-J control groups consider standard polymer separators and Dreamweaver gold and silver separators
  - Some of the 3.35 Ah LG 18650 cells and Molicel 18650-J cells had the NASA/NREL developed internal short circuiting (ISC) devices installed to examine TR behavior at lower temperatures (i.e. closer to field failure conditions); image below depicts the device
  - All cells were tested at 100% state of charge
- **Most experiments are conducted with high flux heaters for a trigger mechanism:**
  - For select cells, some of the FTRC experiments were conducted with nail penetration as well

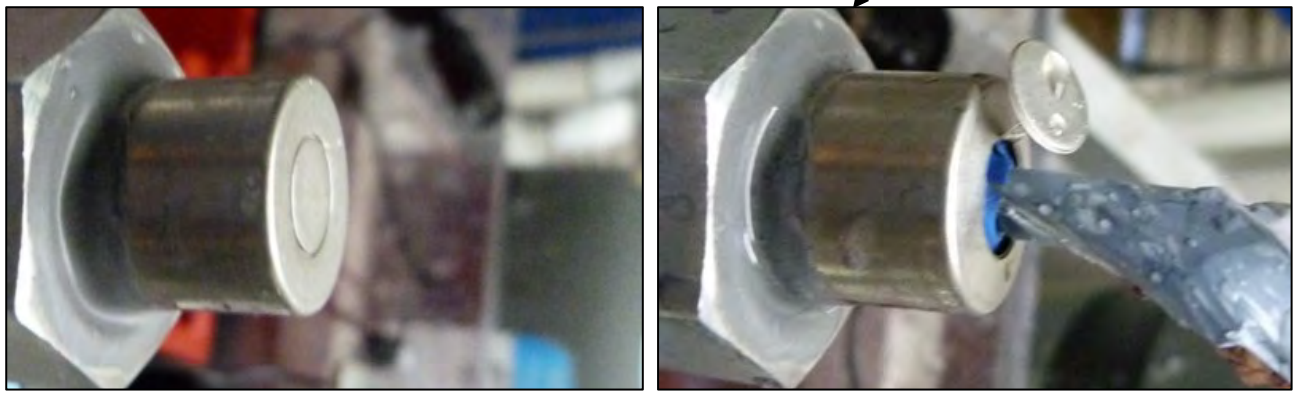
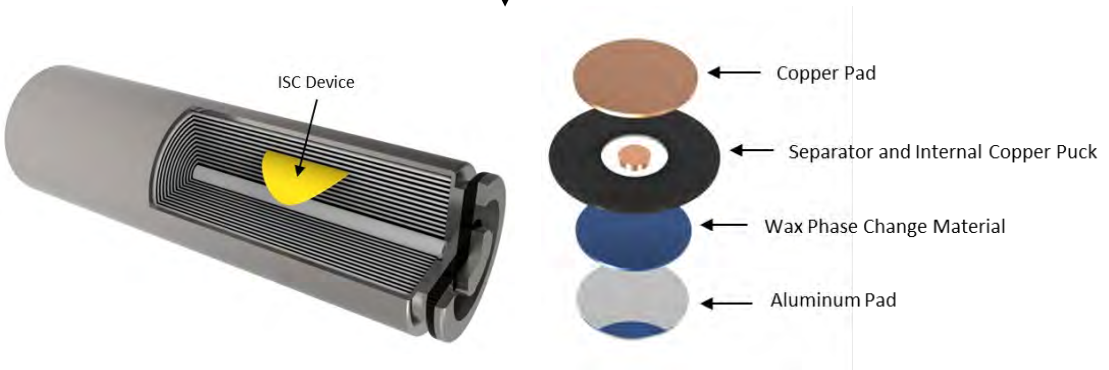


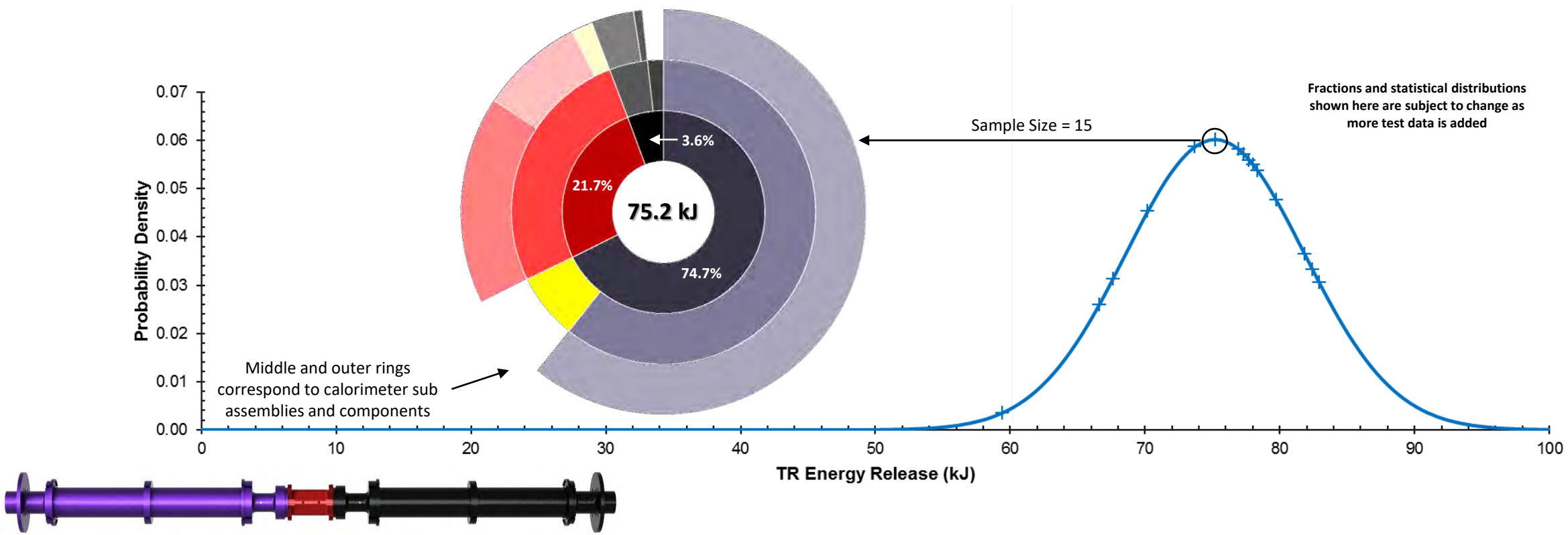
Image courtesy of Darcy, E., et. al. [10]



35 Darcy, E., et. al., S&T Meeting, San Diego, CA. (2016).

LG 18650-MJ1 FTRC RESULTS

- **The LG 18650-MJ1 has violent TR eruptions and consistently releases a large fraction of the total TR energy through the ejecta material and gases (typically on the order of 80%):**
  - Although more violent, less energy may be directed to the neighbor cells depending on failure mechanism
  - The average TR energy release for the LG 18650-MJ1 is 75.2 kJ (standard deviation of 6.6 kJ) where 21.7% is released through the cell casing, 74.7% through the positive side ejecta and gases, and 3.6% through the negative side ejecta and gases

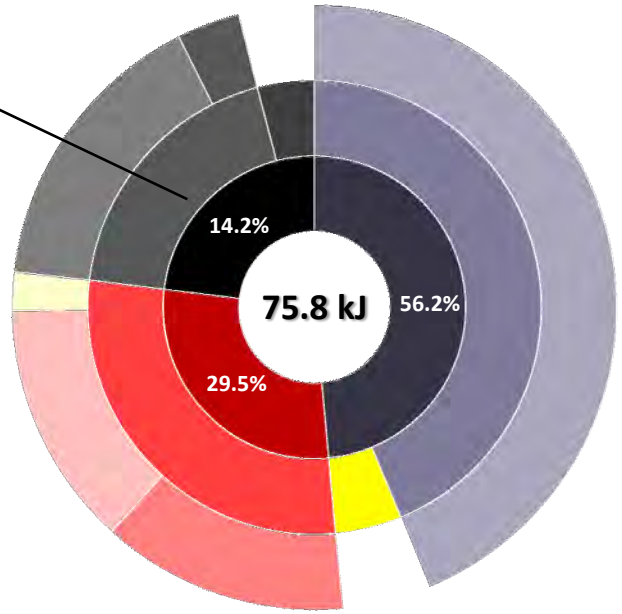


LG 18650-MJ1 FTRC RESULTS

- **The average energy release fractions described on the previous chart are based on all LG 18650-MJ1 results, which include experiments that resulted in bottom ruptures (i.e. off-nominal TR failure mechanism):**
  - The fractions change significantly when consideration is given to the effects of bottom rupture failure mechanisms
  - The figures below show the average energy release fractions associated with bottom rupture (left) vs. non-bottom rupture (right)
  - Results indicate that off-nominal failure mechanisms could be linked with higher total energy release



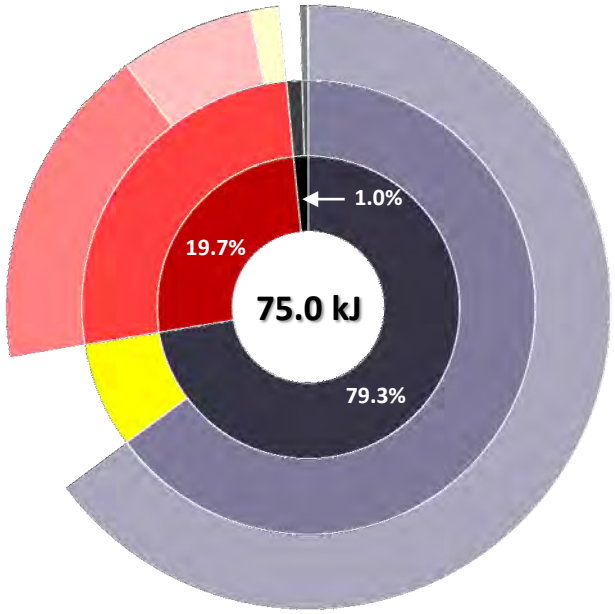
Sample Size = 3



Bottom Rupture
Average Distribution

Middle and outer rings correspond to calorimeter sub assemblies and components

Fractions and statistical distributions shown here are subject to change as more test data is added



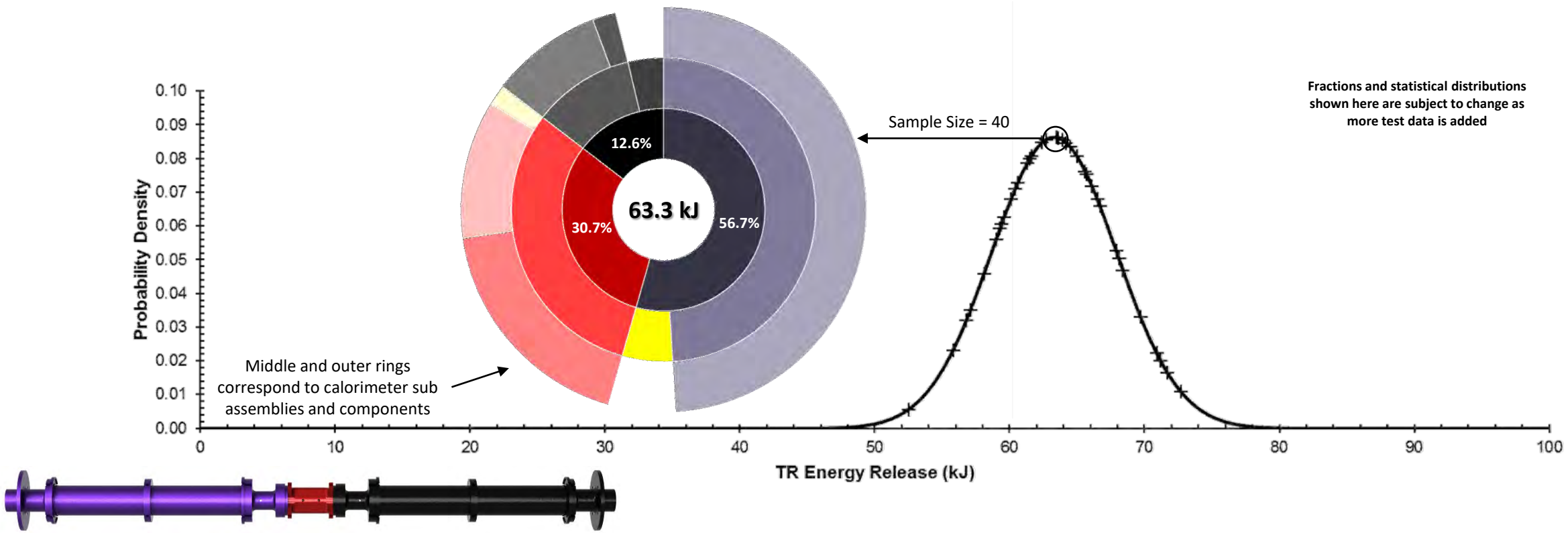
Sample Size = 12

Non Bottom Rupture
Average Distribution



3.35 AH LG 18650 TEST CELL FTRC RESULTS

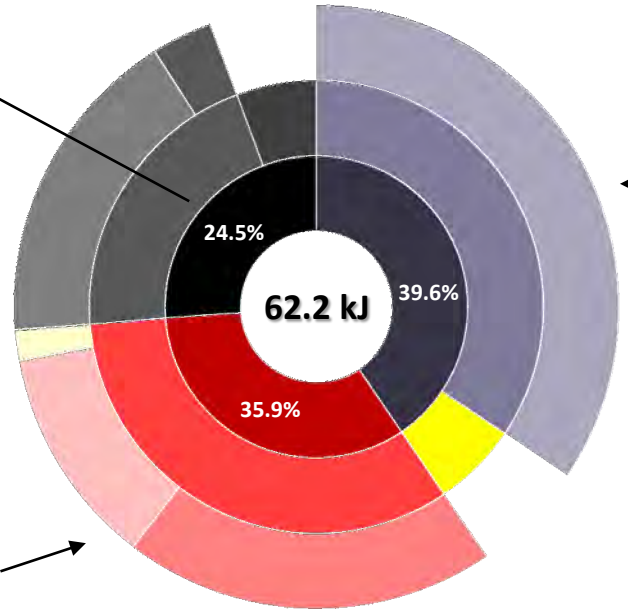
- **The distribution of total TR energy release and the average energy release fractions for all 3.35 Ah LG 18650 tests (regardless of cell configuration) are shown below:**
  - The average TR energy release for the 3.35 Ah LG 18650 is 63.3 kJ (standard deviation of 4.6 kJ) where 30.7% is released through the cell casing, 56.7% through the positive side ejecta and gases, and 12.6% through the negative side ejecta and gases
  - We know intuitively that fractions presented below are skewed due to averaged BV and NBV results



3.35 AH LG 18650 TEST CELL FTRC RESULTS

- **Processing data with consideration given to BV vs. NBV cells shows some interesting results:**
  - BV cells had a slightly lower standard deviation for total TR energy release (2.8 kJ vs. 4.2 kJ for NBV)
  - BV cells transfer higher proportion of heat through the cell casing compared to the NBV cells
  - NBV cells had a higher magnitudes of total TR energy release
  - Possibly due to the increased "violence" associated with non-BV TR events



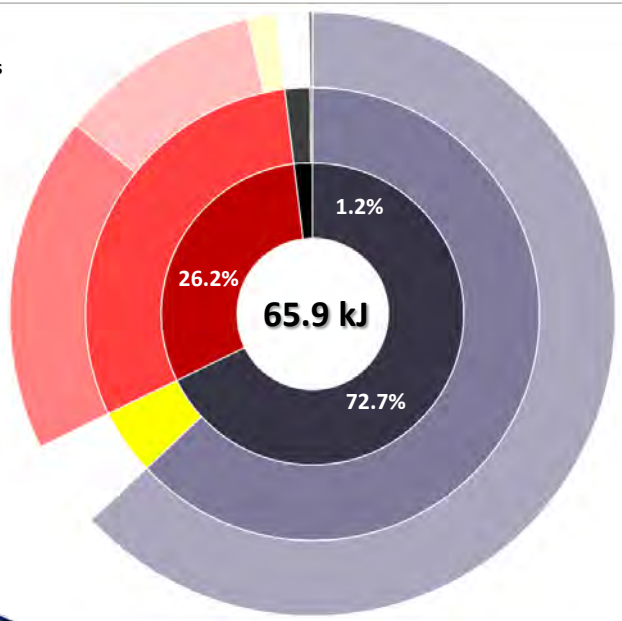


Middle and outer rings correspond to calorimeter sub assemblies and components

Fractions and statistical distributions shown here are subject to change as more test data is added

Sample Size = 16

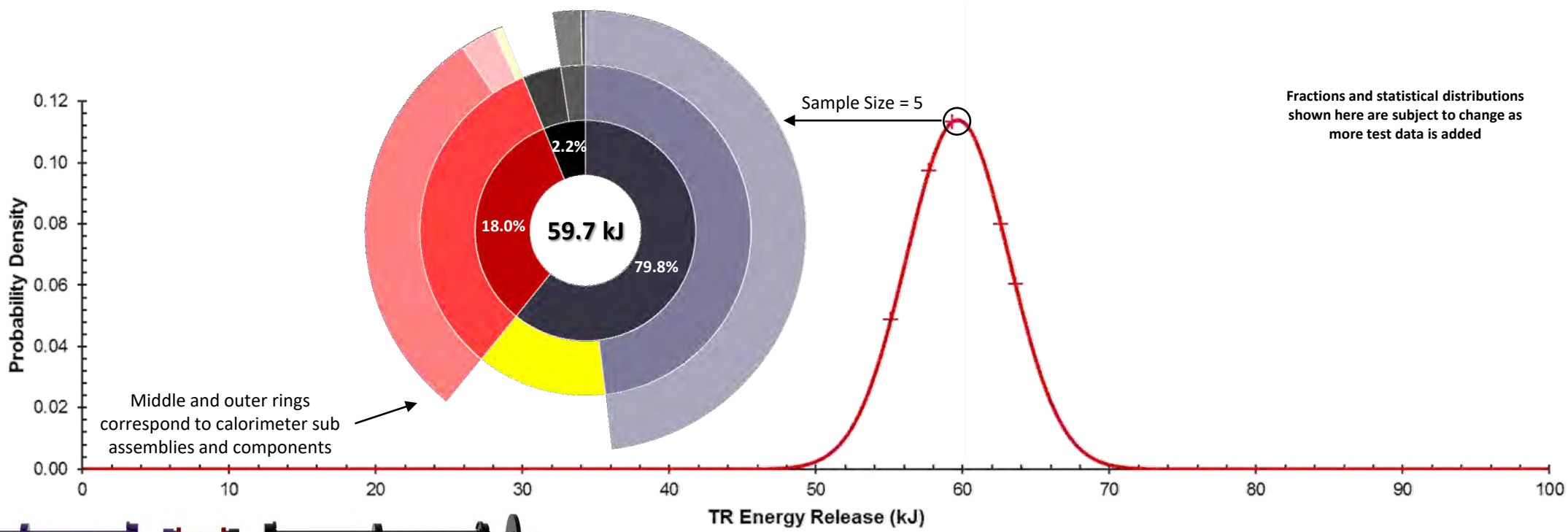
Sample Size = 16





SAMSUNG 18650-30Q FTRC RESULTS

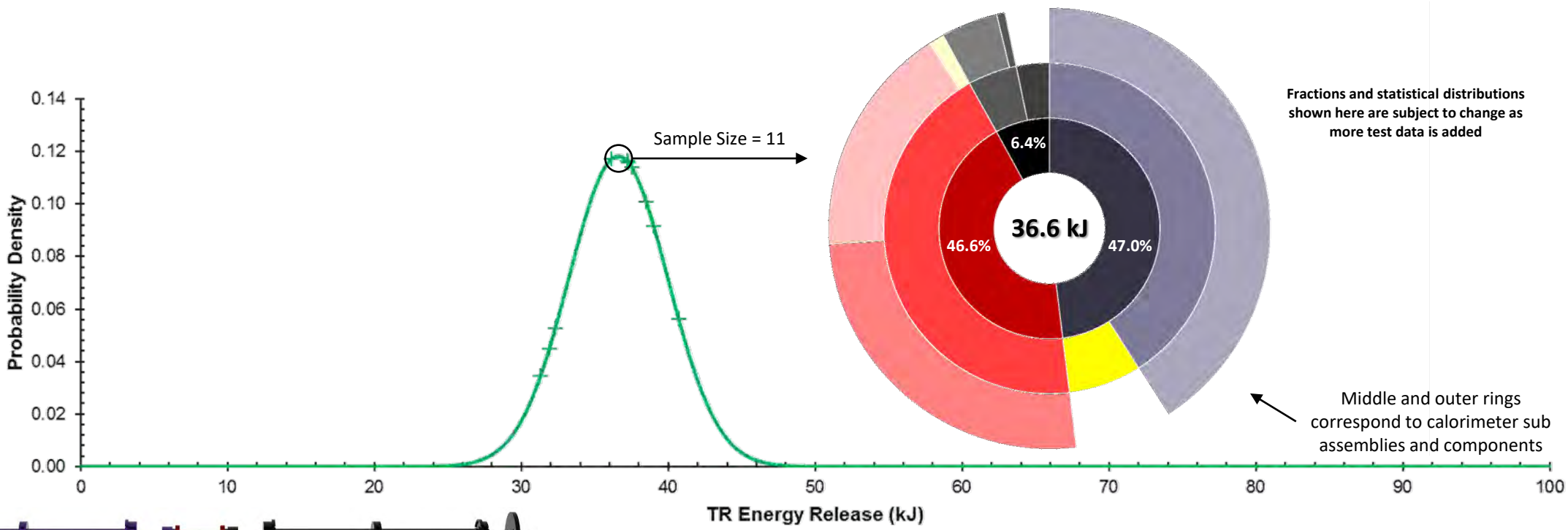
- **Only 5 calorimetry experiments conducted so far for the Samsung 18650-30Q:**
  - Efforts in work to conduct 5 more tests to complete the assessment of the cell
  - The average TR energy release for the Samsung 18650-30Q is 59.7 kJ (standard deviation of 3.5 kJ) where 18.0% is released through the cell casing, 79.8% through the positive side ejecta and gases, and 2.2% through the negative side ejecta and gases





MOLICEL 18650-J FTRC RESULTS

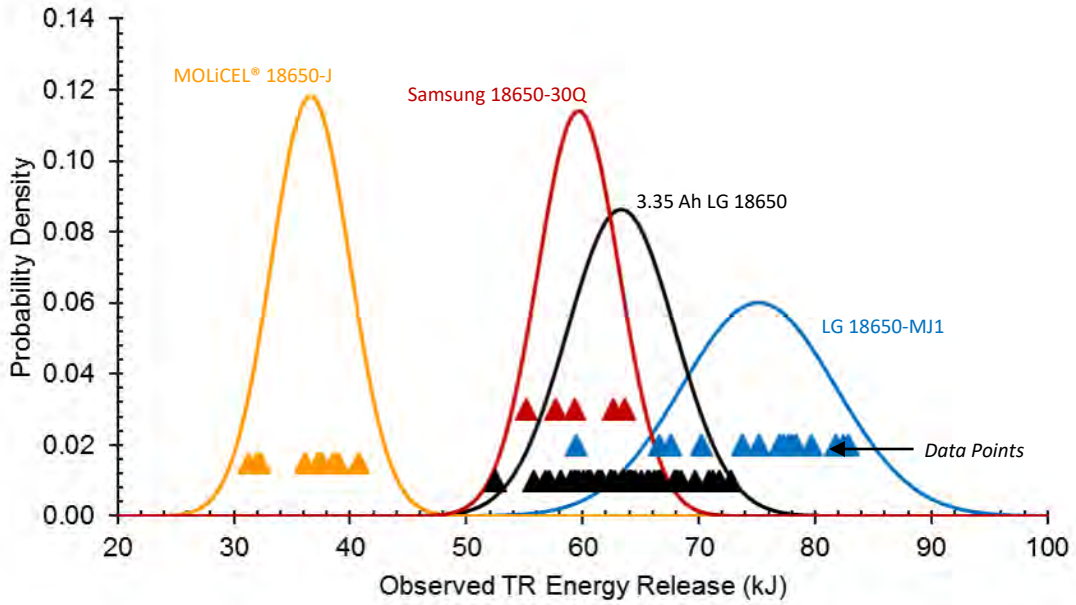
- **The distribution of total TR energy release and the average energy release fractions for all Molicel 18650-J tests (regardless of cell configuration) are shown below:**
  - Three proprietary separator materials were considered in the tested cells which could contribute to the test-to-test variance
  - The average TR energy release for the Molicel 18650-J is 36.6 kJ (standard deviation of 3.4 kJ) where 46.6% is released through the cell casing, 47.0% through the positive side ejecta and gases, and 6.4% through the negative side ejecta and gases
  - Least violent of all cell designs tested, but has the highest proportion of heat transferred through the cell casing

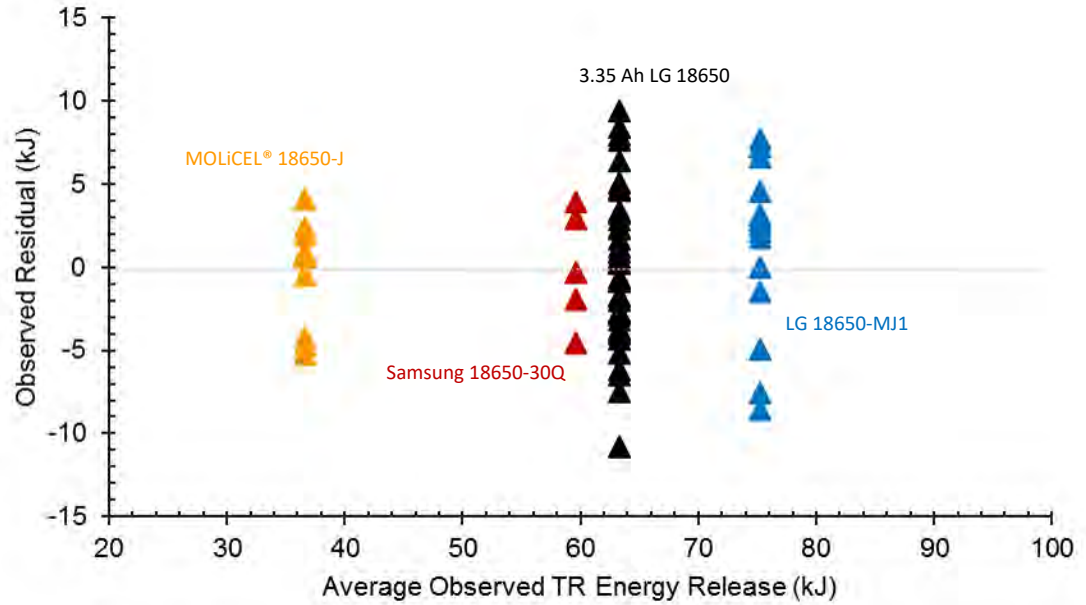




COMPARING TOTAL ENERGY RELEASE

- **Higher energy cells (e.g. the LG 18650-MJ1) release more TR energy, have more violent ejections, and lower remaining cell mass when compared to lower energy cells (e.g. the Molicel 18650-J):**
  - Note that the normal distributions (left image) shown below are created from the raw data and are generated to give an initial glance at the data
  - The residuals shown below (right image) are based on the raw data and reflect the difference between the observed value and the average value
  - These plots do not break down the impacts of the aforementioned design variables on the thermal runaway behavior; hence the significant differences in standard deviations and residual spread as seen the plots below
  - Although direct interpretation of the raw data is insightful, we recommend referring to the regression model results (next few slides) for final assessment of thermal runaway behavior





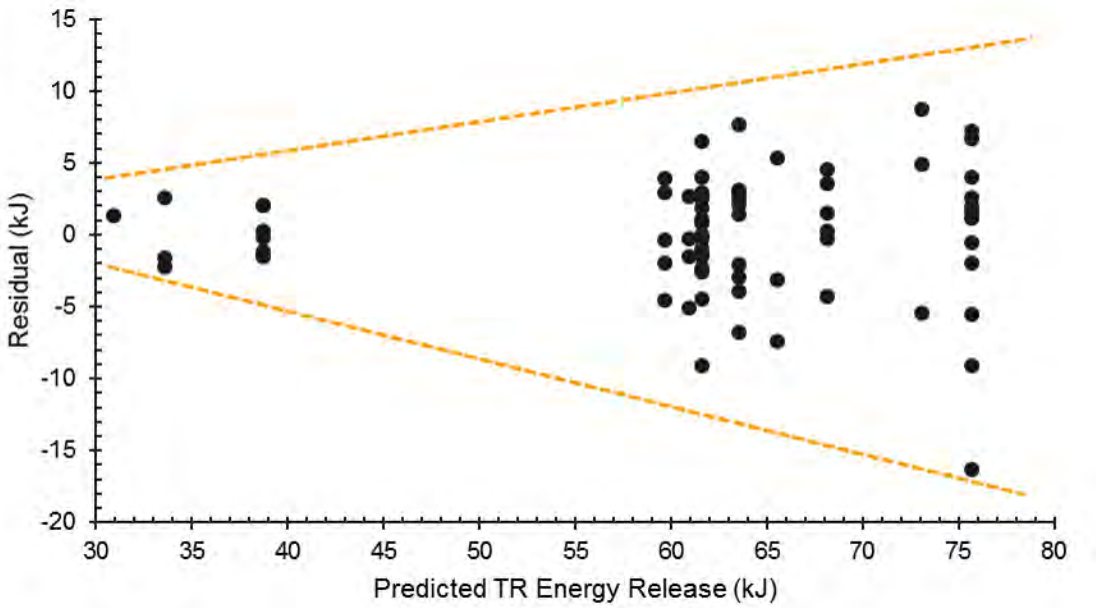
Images submitted to J. Power Sources August 2018

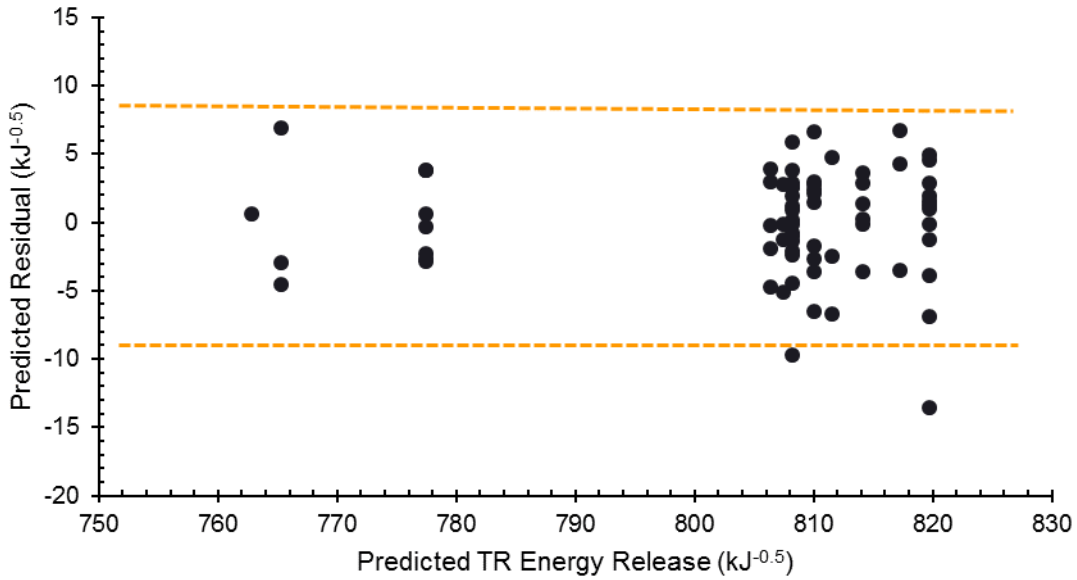
ENGINEERING STATISTICS METHODOLOGY

- **Special thanks to our NESC statistician Kenneth Johnson who developed the regression model discussed here**
- **The TR results for each experiment are directly post-processed with primary consideration given to the following:**
  - Total TR energy yield
  - Fraction of energy released through the cell casing vs. through the ejecta materials and gases
  - Remaining cell mass following TR
  - The raw data derived versions of these values are referred to as the “observed” values and serve as inputs to a regression model
- **No two TR events are identical which results in variation of total TR energy release on a test-to-test basis:**
  - This variation is a function of various random and non-random factors associated with the experiments
  - A regression model was developed as a function of all of the FTRC results (e.g. cell type, failure mechanism, energy distribution, total energy release)
  - The completed regression model then uses the observed values for each experiment and outputs a corresponding predicted total energy release
  - The predicted energy release values are then used to recreate distributions to characterize the range of thermal runaway energy release
- **Note that the regression model can be used to predict energy fractions as well, but at this point we are only using it to predict total energy release:**
  - The predicted values and the associated distributions are shown on the next few slides

PREDICTED TOTAL ENERGY RELEASE

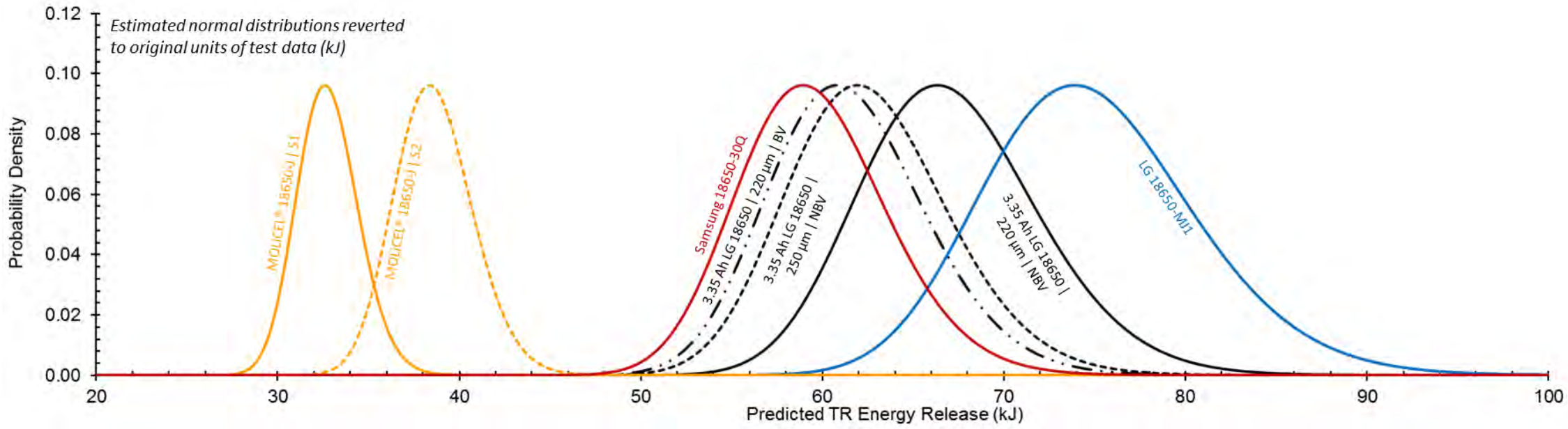
- **First it is important to examine how effective the regression model is at predicting total energy release:**
  - This effectiveness can be considered by looking at the residuals (differences between predicted and corresponding observed values)
- **A key assumption for the regression analysis was equal variability of the residuals across zero:**
  - Residual = difference between predicted value and corresponding observed value
  - Initial model, based on total energy release in kJ, did not satisfy this assumption (left image)
  - Performed inverse-square root translation of observed total energy release ($kJ^{-0.5}$) factor to achieve a better model (right image)





PREDICTED TOTAL ENERGY RELEASE

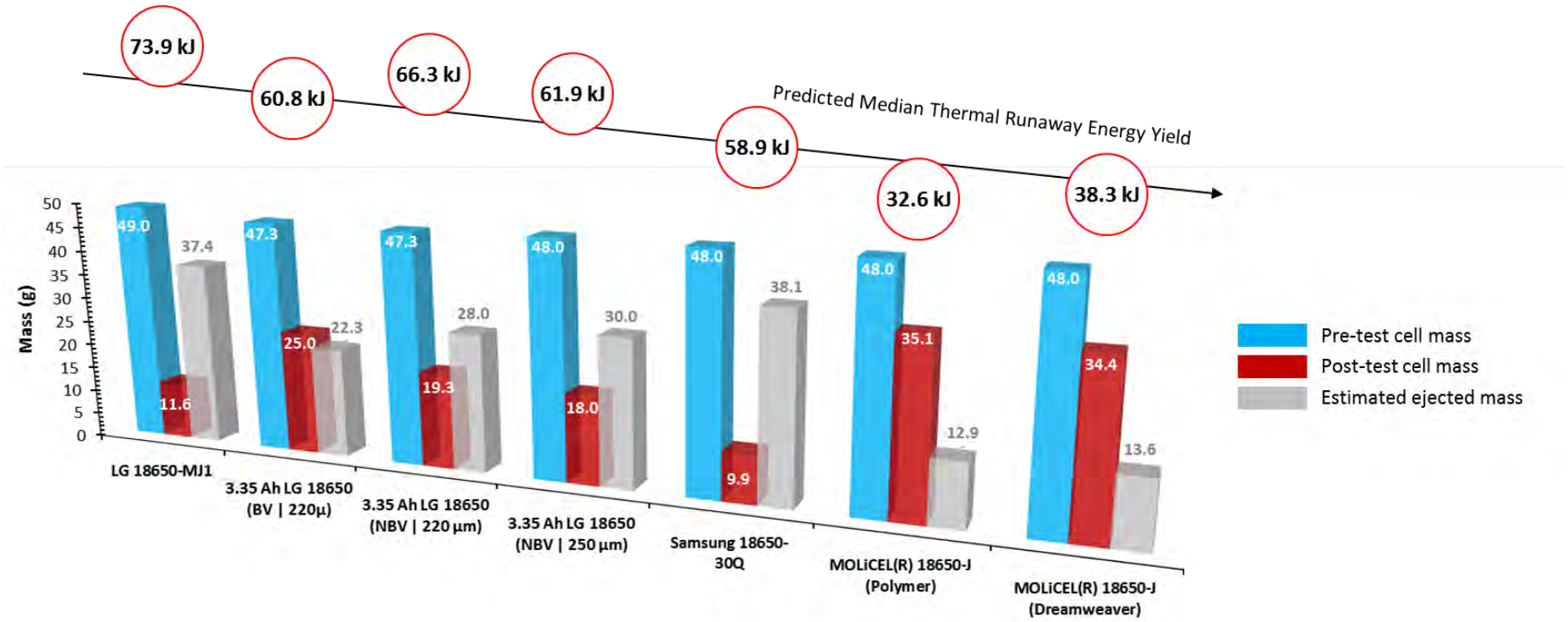
- **Final regression model results for total energy release were in inverse square root units (kJ $^{-0.5}$) as seen on the previous slide:**
  - These predictions were then translated back into the original units (kJ) for final interpretation
- **Distributions based on the final predicted values (in kJ) were then created:**
  - Think of the distribution curves below, plus the previously shown fractional pie charts, as the end goal for every cell, cell configuration, and cell variable that we attempt to characterize
  - The power of the regression model becomes apparent as we are now able to analyze the impacts of the random and non-random variables on thermal runaway behavior



Images submitted to J. Power Sources August 2018

POST THERMAL RUNAWAY MASS COMPARISON

- **BV cells consistently release less heat and have higher remaining cell mass than NBV cells:**
  - Having two pressure relief points in BV cells helps reduce the pressure drop between inside the cell and outside, leading to a lower driving force for materials to eject. Hence BV cells have a higher remaining mass
  - There is evidence of a relationship between total mass loss and the heat released during thermal runaway. This may be due to the decomposition reactions being oxygen limited, where less active material is ejected and hence less material is in an oxygen-rich environment suitable for thermal runaway
  - Results indicates a less severe and more predictable TR event as an effect of the BV feature

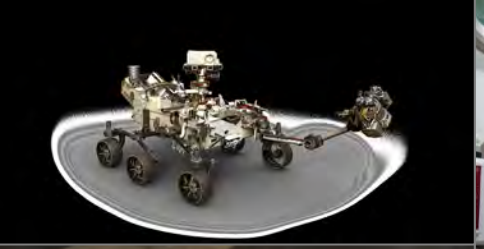


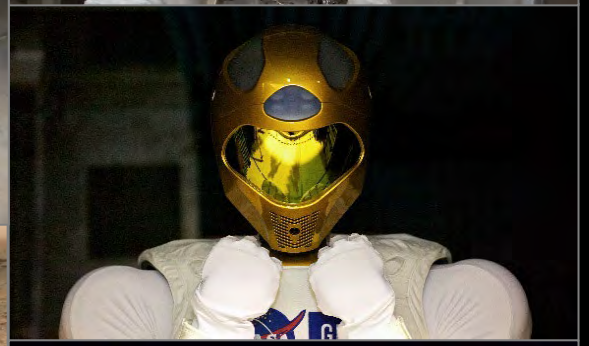
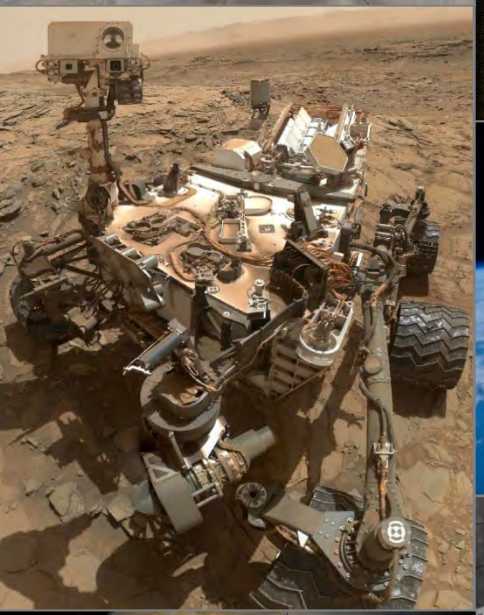
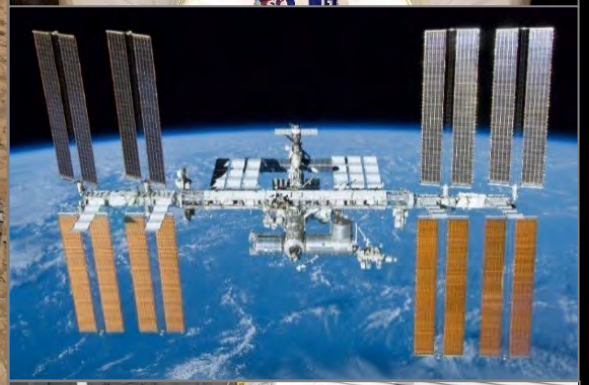
SUMMARIZING THERMAL RUNAWAY VARIANCE

- **This new calorimetry method, and the associated results, enables the discernment of the fractions of TR energy released through the cell casing and through the ejecta material:**
  - Due to the variability in thermal runaway responses, we recommend at least 10 runs to establish statistically defendable results
  - Can analyze the spread of heat sources when cells rupture and compare to when they remain intact
- **Results provide the means to develop optimized Li-ion batteries while also maintaining safety and margin**
- **Higher energy cells produce more heat and eject more material during TR:**
  - Higher magnitudes of total energy released and more violent ejections
  - Less energy associated with the cell body and more energy associated with the ejecta
  - The correlation is not very linear because cell enclosure design impacts the results
- **BV cells consistently released less TR energy (~4 kJ for 3.35 Ah LG cell) and have higher post TR cell mass than non-BV cells:**
  - BV cells produce less and more localized heat, hence a less severe and more predictable TR event as an effect of the BV feature
  - Battery designers should be ready to accommodate and take advantage of cell designs with the BV feature in the future

CURRENT FOCUS OF FTRC EFFORTS

- **The current focus of the FTRC efforts is on characterizing TR behavior for nail induced TR, ISC TR, and heater induced TR**
- **Examining the effects of failure location on rupture behavior using the ISC device**
- **Development of accommodations for small format cells beyond 18650 cells**
  - 21700 cells
  - D-Cells
  - Pouch cells
- **Development of FTRC capability for >100 Ah Li-ion cells**
- **Improvement of regression modeling techniques**

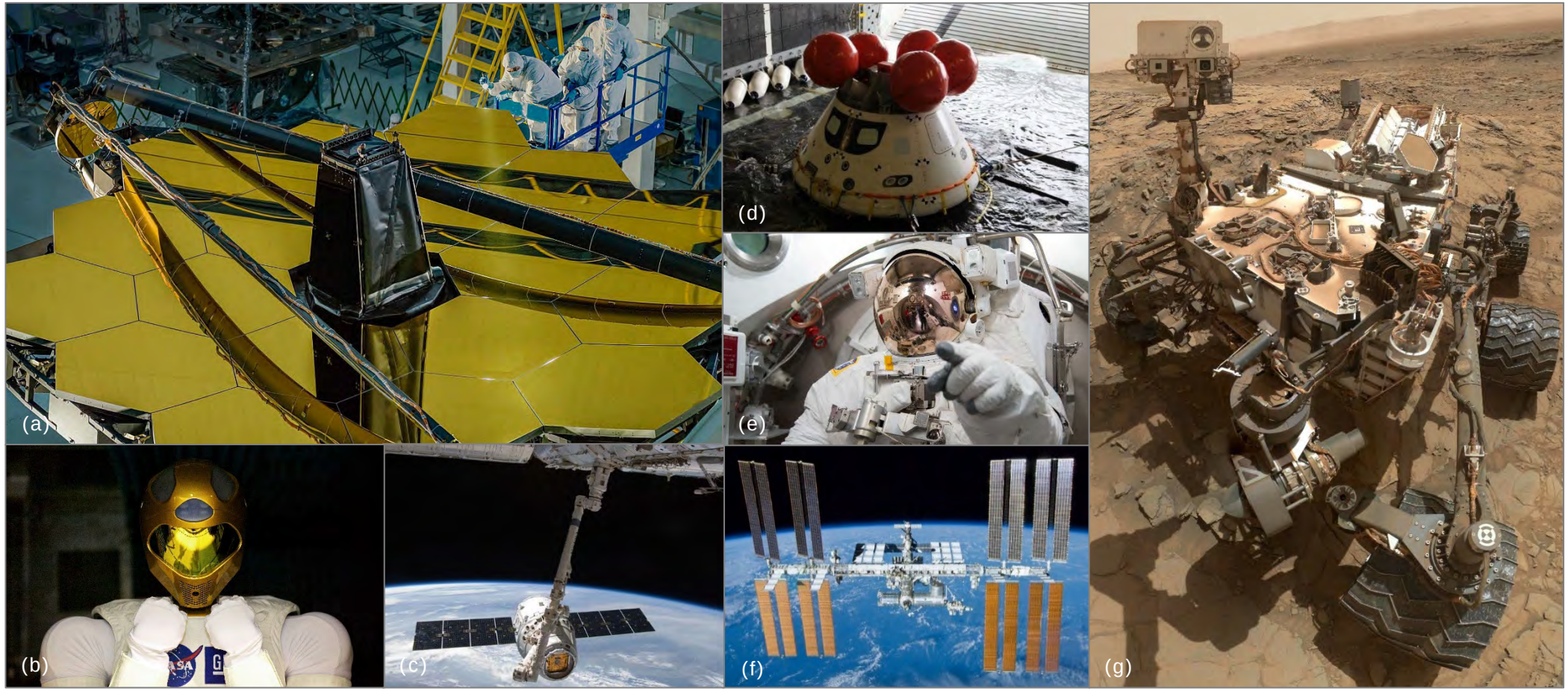




MODULE 2 SECTION 5:
NASA'S RESPONSE TO THERMAL RUNAWAY

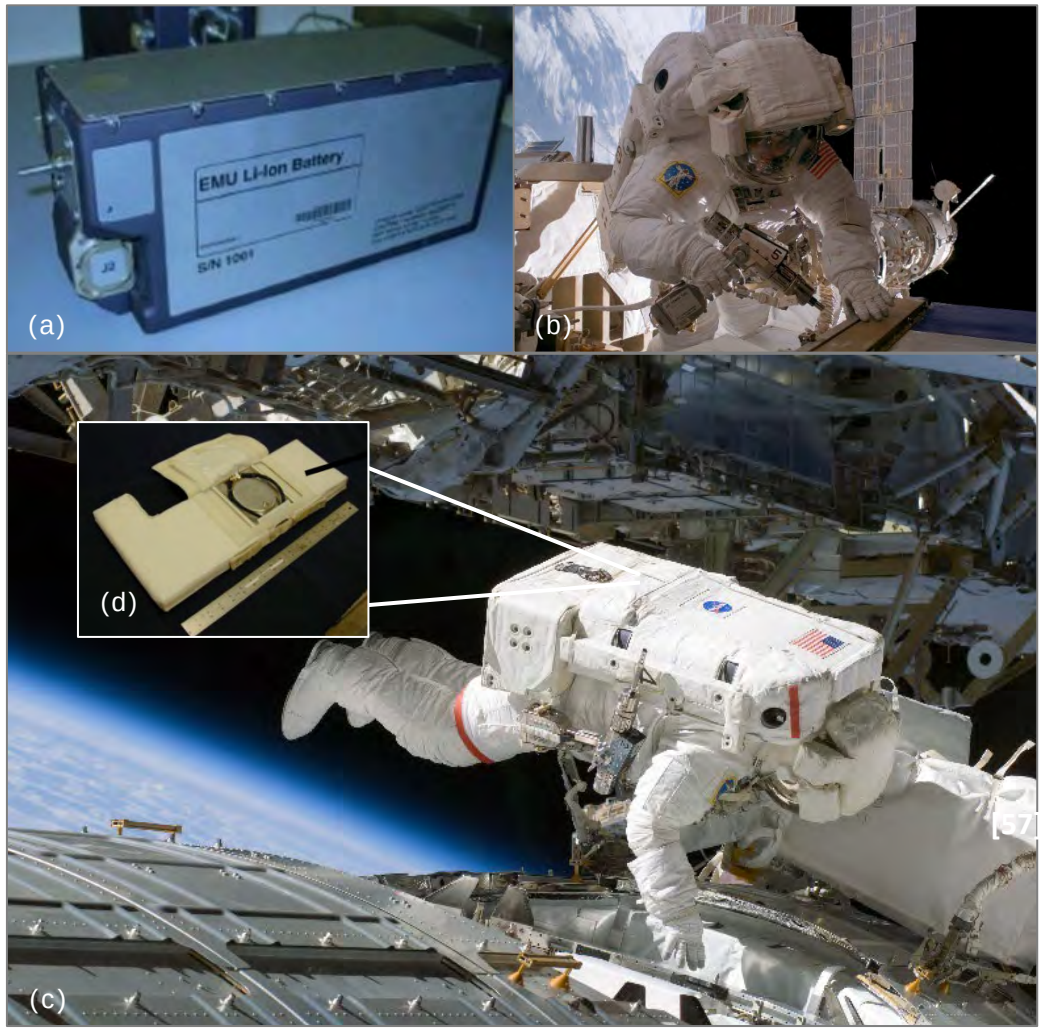
SPACE APPLICATIONS THAT USE LITHIUM-ION BATTERIES



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, expect for image (e) where credit is given to the US Navy.

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:**
  - Li-ion Rechargeable Extravehicular Activity battery assembly (LREBA)
  - Li-ion Pistol Grip Tool battery assembly (LPGT)
  - Long Life Battery (LLB) for EMU
- **NASA and NESC provide new 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:**
  - 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

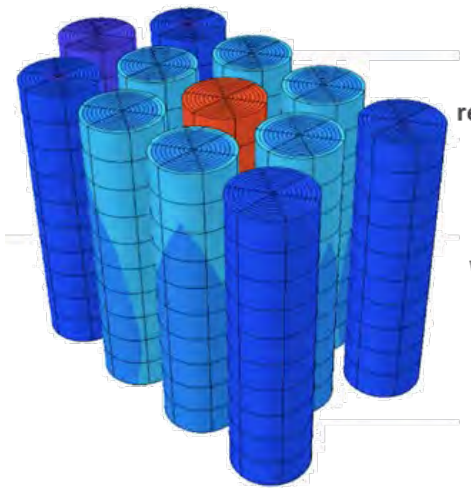


Public access images representing the EMU Li-ion batteries evaluated by the NESC: (a) LLB, (b) LPGT, (c) EMU LREBA image 1, (d) EMU LREBA image 2.

36 Darcy, E., et. al., Advanced Automotive Battery Conference (2017).

NASA'S RESPONSE TO THERMAL RUNAWAY

- **Development of optimized Li-ion battery assemblies that satisfy the aforementioned strategies requires knowledge of the following TR characteristics:**
  - Total energy output range during TR for a single Li-ion cell
  - Fraction of TR energy transferred through the cell casing
  - Fraction of TR energy ejected through cell vent/burst paths



How much heat do I need to remove from the local system?

How do I support the design with thermal analysis?

What is my simulated energy distribution?



How do I best protect the adjacent cells with minimal additional mass / volume?

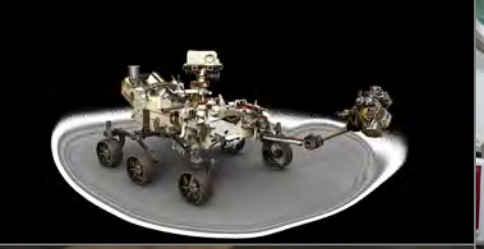
What works best? A heat sink, interstitial foam or a combination?

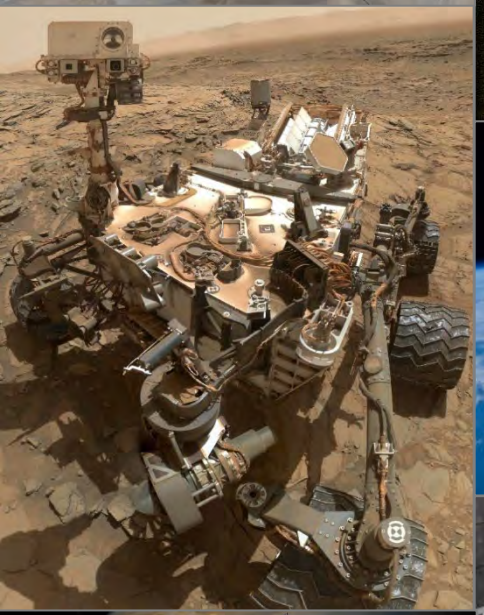
Is an interstitial material needed for thermal protection?

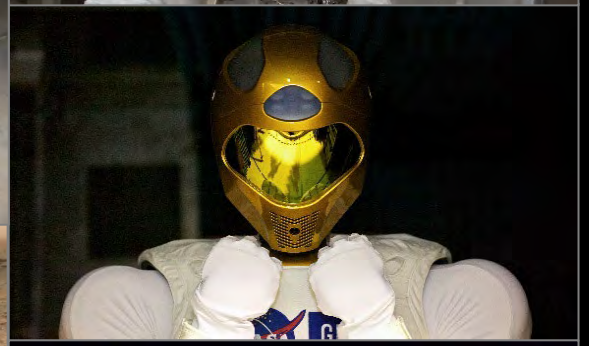
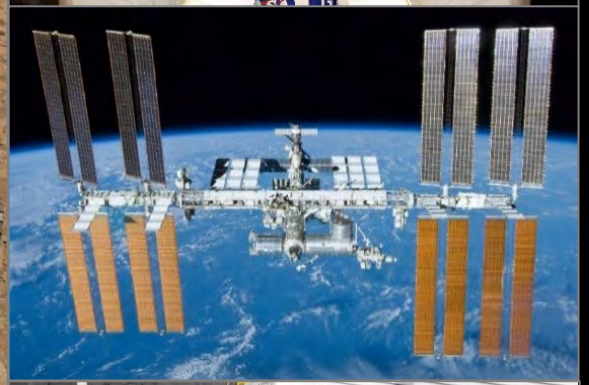
How far about should the individual cells be spaced?

What cell should be selected?

36 Darcy, E., et. al., Advanced Automotive Battery Conference (2017).






MODULE 2 SECTION 6:

SAFE BATTERY DESIGN RELATED LESSONS LEARNED

LESSONS LEARNED

- Design must prevent first TR propagation from initial failed cell
- Limiting cell to cell thermal conduction appears to help prevent cell-to-cell propagation
- Maximizing heat conduction between cells and enclosure may also help prevent cell-to-cell propagation
- Parallel cell bussing can provide significant in-rush currents into failed cell, which gets them hot
- Radiative energy transfer alone is not the dominant contributor to cell-to-cell propagation
- Combustion of expelled electrolyte must directed away from adjacent cells
- Ejecta material can bridge to adjacent cells and cause cascading short circuiting
- It is imperative to control vented/ejected products

36 Darcy, E., et. al., Advanced Automotive Battery Conference (2017).

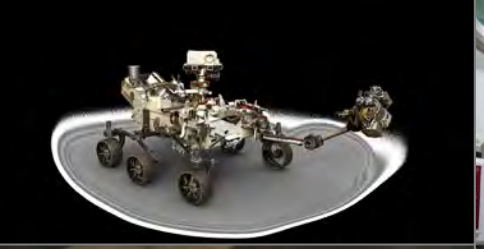
Credit: Eric Darcy

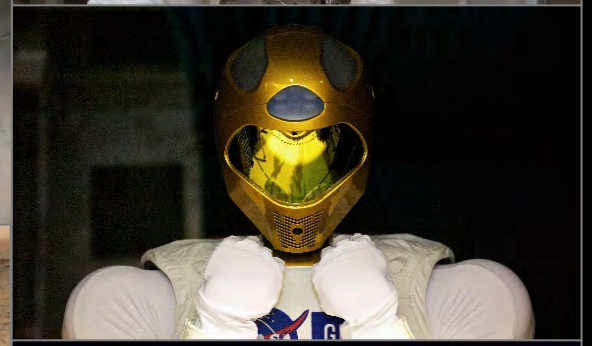
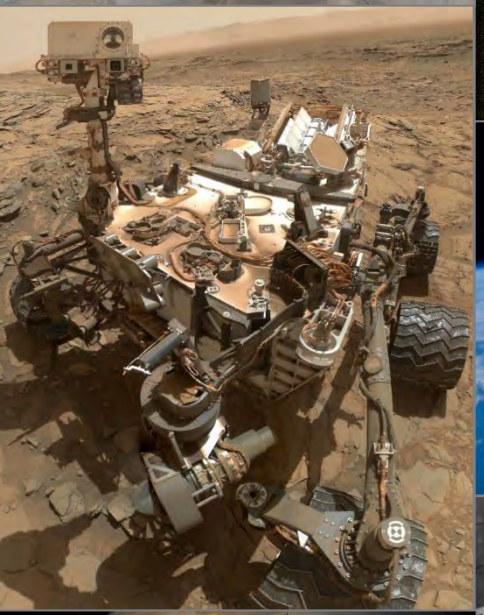
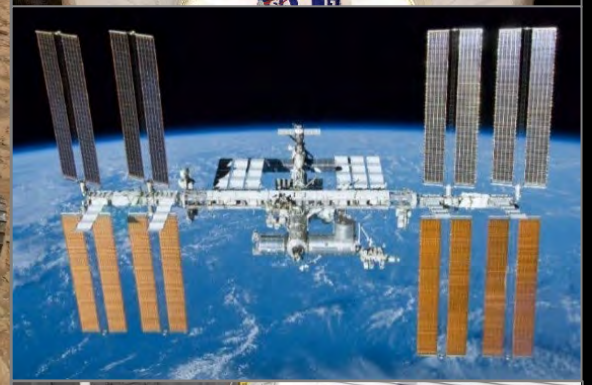
LESSONS LEARNED

- **Compliance with the following rules can help prevent cell-to-cell propagation:**
  - Minimize side wall ruptures
  - High thermal conductivity interstitial heat sinks
  - No direct cell-cell contact; direct contact nearly assures propagation
  - 0.5mm cell spacing can work, but spacing out cells > 1mm is very beneficial
  - Individually fusing cells in parallel
  - Protect adjacent cells from ejecta materials (all solids, liquids, and gases)
- **Include flame arresting vent ports to minimize combustion effects:**
  - Create tortious path with flame arresting screens
- **Some high energy density (>600 Wh L^{-1}) are very likely to experience side wall ruptures during TR**
  - Structural syntactic foams or steel tubes work
- **Corner and edge cells are more vulnerable than interior cells towards TR propagation**
- **Ejecta is electrically conductive and can cause circulating currents**
- **Entire battery gets hotter with each subsequent cell TR event**
- **Soft goods bag and conductive absorptive material prevent exiting flames**
- **Subscale test results can be misleading and no replacement for full scale test verifications**

36 Darcy, E., et. al., Advanced Automotive Battery Conference (2017).

Credit: Eric Darcy



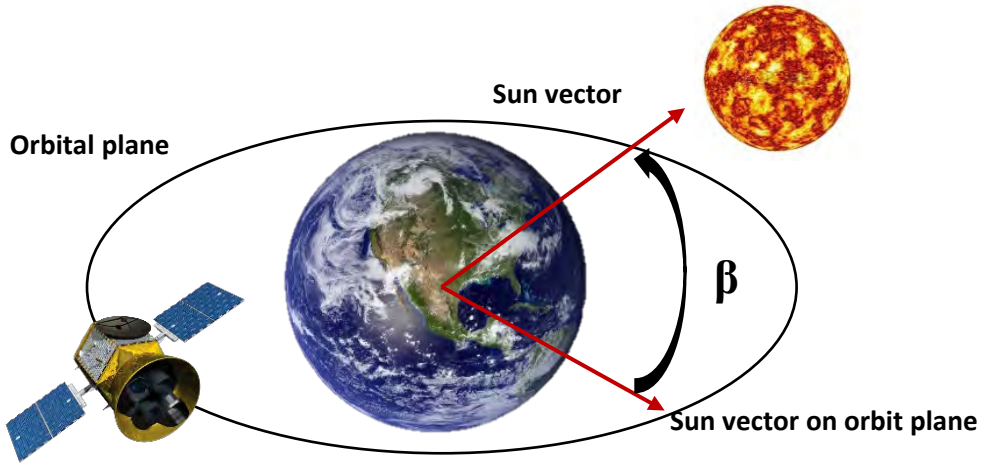


MODULE 3 SECTION 1:

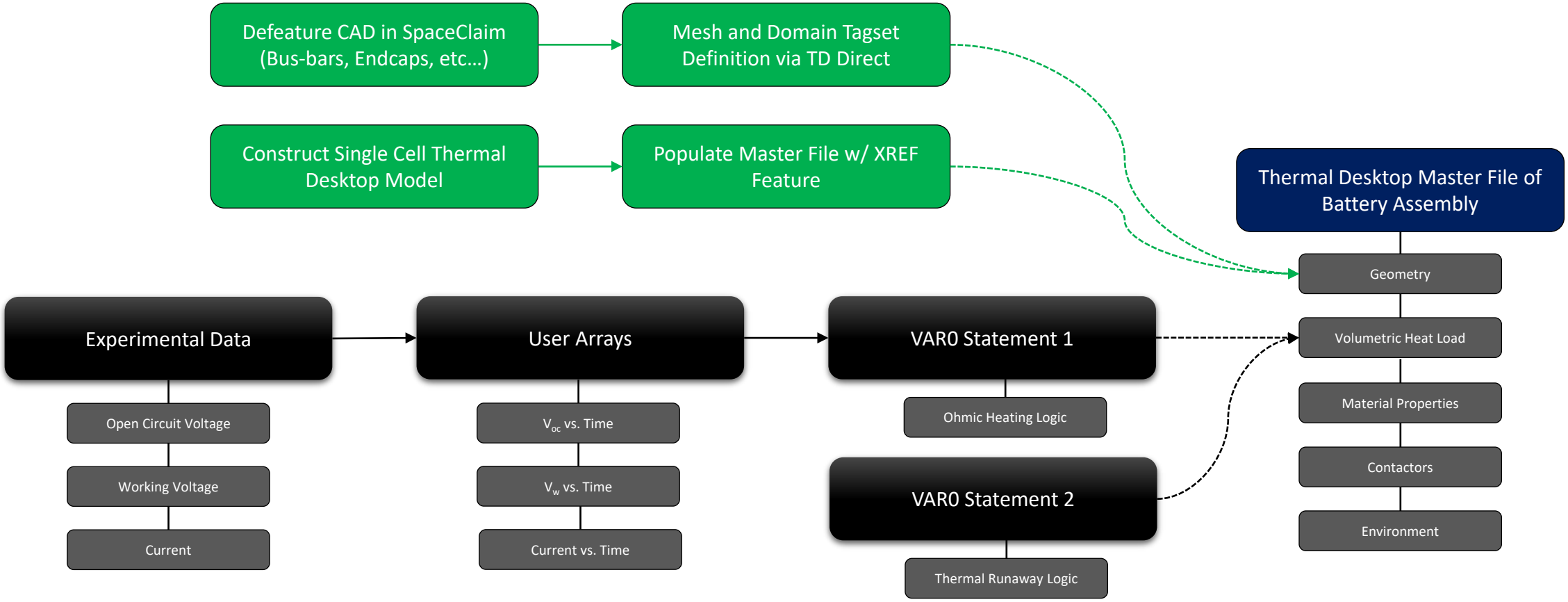
PRACTICAL THERMAL MODEL CONSTRUCTION TECHNIQUES

PRACTICAL THERMAL MODEL CONSTRUCTION TECHNIQUES

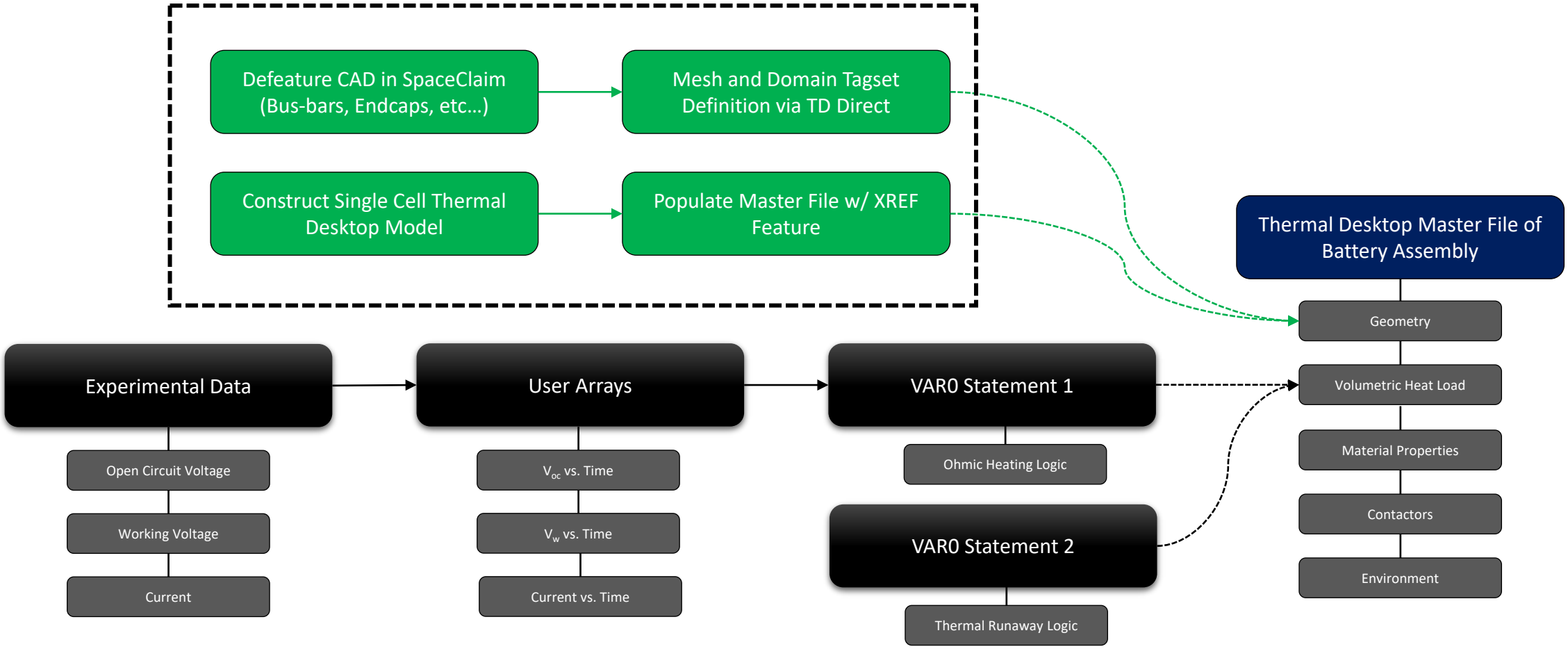
- **Li-ion battery performance, efficiency and safety are heavily influenced by cell temperature and surrounding temperature**
- **Accurate prediction of Li-ion battery thermal performance requires test-correlated thermo-electrochemical models:**
  - Generally, the optimal way to perform thermo-electrochemical analysis is with a multiphysics methodology, however;
  - Non-multiphysics software that support user-defined heat loads and variable statements can do the trick
- **Here we use a 14-cell example to demonstrate methods to quickly develop thermal models of battery assemblies via SpaceClaim, TD Direct and Thermal Desktop:**
  - Users may have access to different software suites, but the principles discussed here should remain the same
  - The intent here is to not be software specific, but rather to be practical in approach
  - FYI… original interest in using software capable of simulating thermal radiation driven environments was a function of my desire to simulate battery heat generation rates as a function orbital environments (which is important when considering the relevant temperature dependencies)



PRACTICAL THERMAL MODEL CONSTRUCTION TECHNIQUES

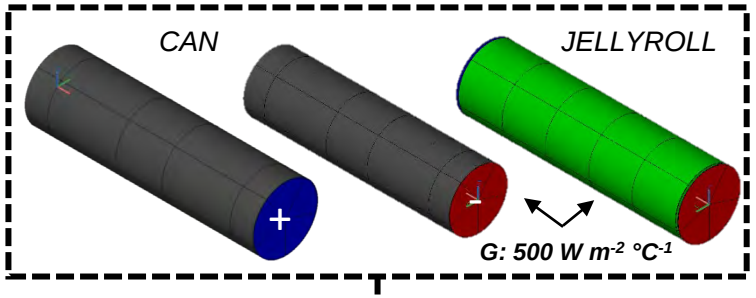


PRACTICAL THERMAL MODEL CONSTRUCTION TECHNIQUES

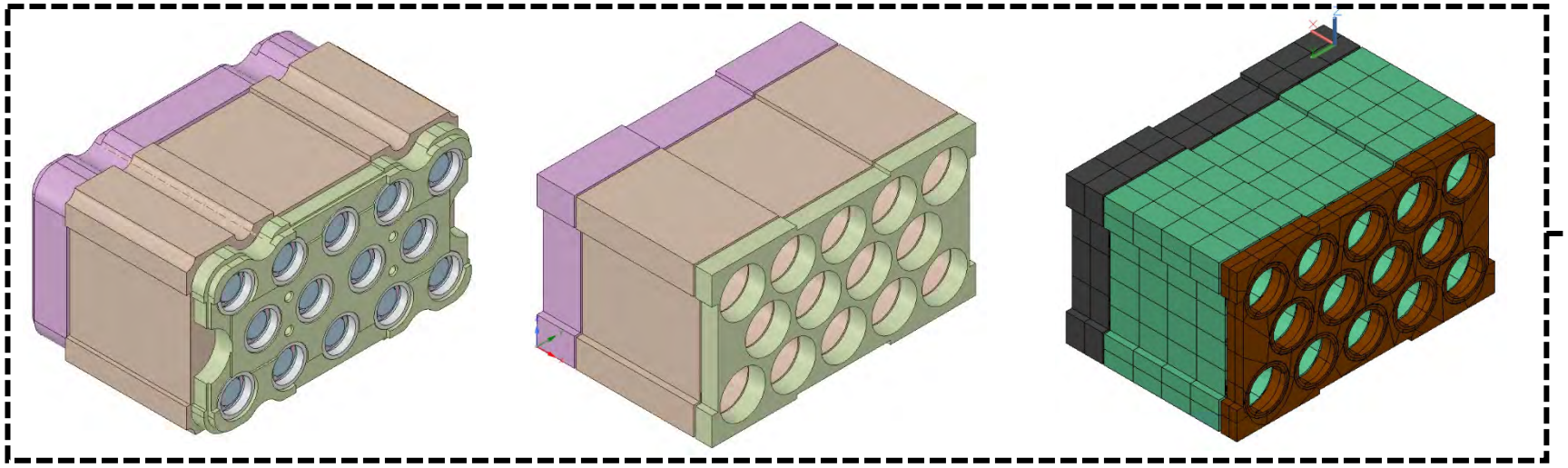


PRACTICAL THERMAL MODEL CONSTRUCTION TECHNIQUES

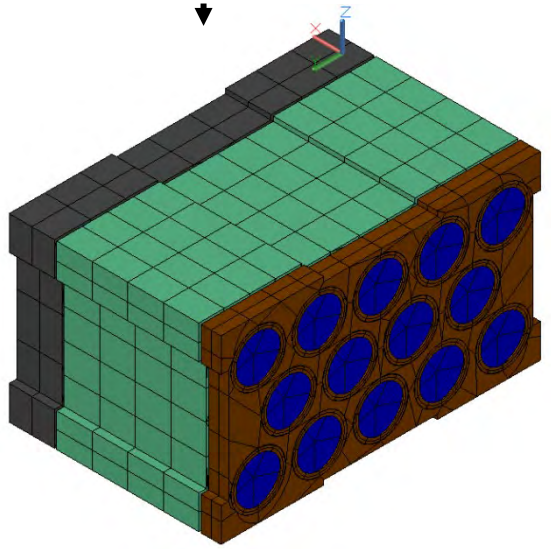
- **Example considers a bank of x14 18650 cells (similar size as AAA cell)**
  - Defeature CAD file of bank geometries via SpaceClaim
  - Create a separate groups for surfaces contacting the cells (contactor will be created later)
  - Separate domain tag sets should be created for any surface contacting 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



PRACTICAL THERMAL MODEL CONSTRUCTION TECHNIQUES

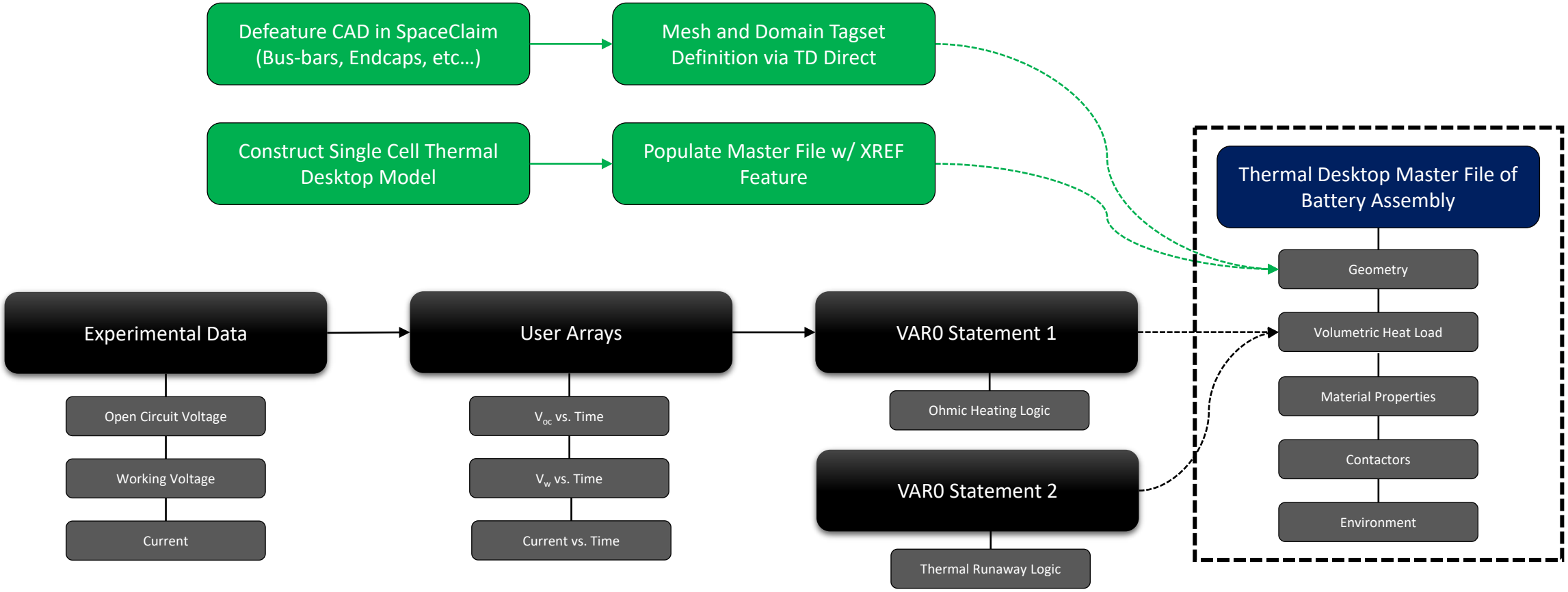
- **Ohmic heat generation may be applied to as a single heat load in the master file of the battery assembly**
  - In the cell reference file, create a domain tag set that contains the jellyroll
  - In the master file, create registers for each of the variables in Bernardi's equation; we will simplify 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**

$$Q_{JELL} = \text{Current} \times \left[V_{OC} \text{ Bivariate Array} - V_W \text{ Bivariate Array} \right]$$

	-45°C	-25°C	0°C	+25°C	+45°C
0min	#	#	#	#	#
10min	#	#	#	#	#
20min	#	#	#	#	#
30min	#	#	#	#	#
40min	#	#	#	#	#
50min	#	#	#	#	#
60min	#	#	#	#	#
70min	#	#	#	#	#

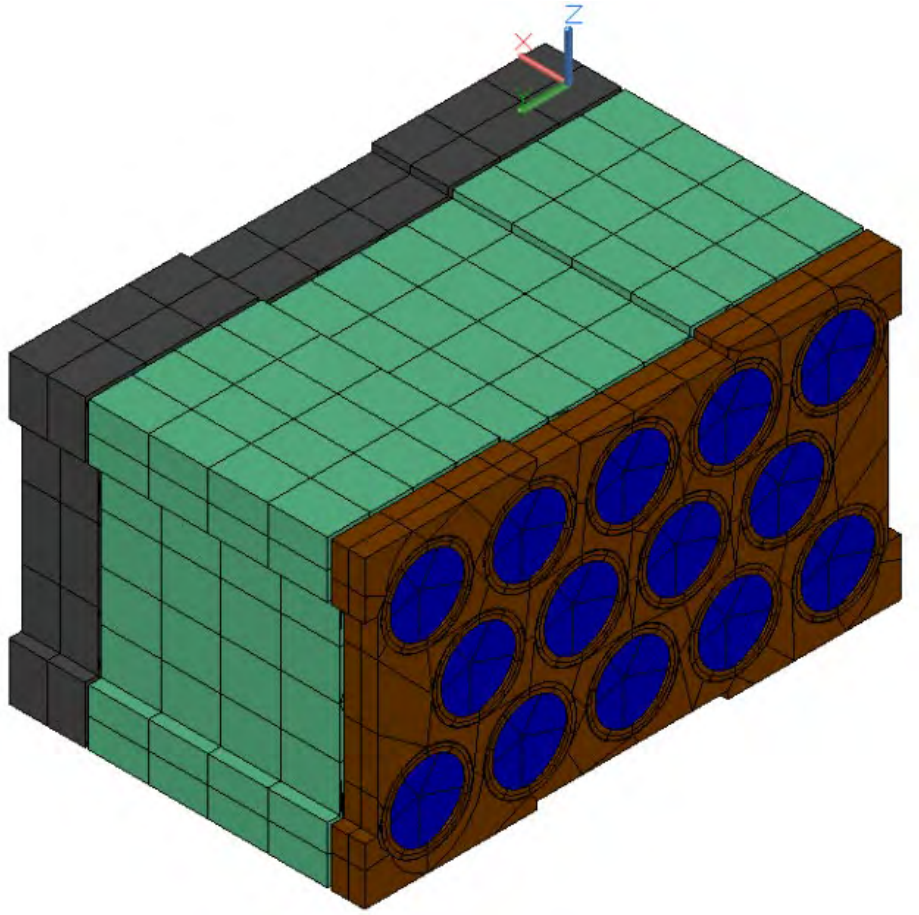
	-45°C	-25°C	0°C	+25°C	+45°C
0min	#	#	#	#	#
10min	#	#	#	#	#
20min	#	#	#	#	#
30min	#	#	#	#	#
40min	#	#	#	#	#
50min	#	#	#	#	#
60min	#	#	#	#	#
70min	#	#	#	#	#

PRACTICAL THERMAL MODEL CONSTRUCTION TECHNIQUES



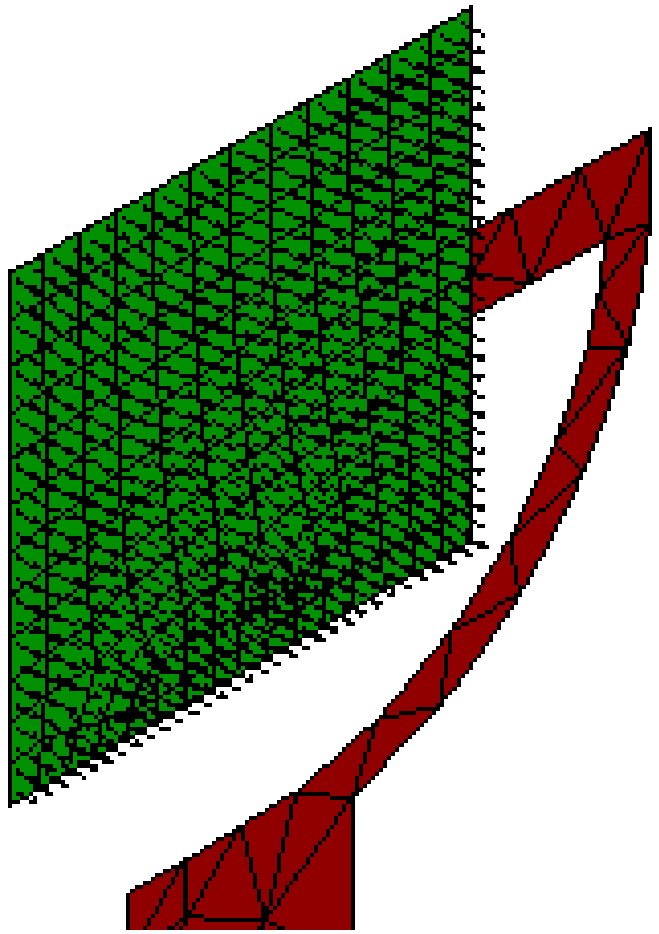
PRACTICAL THERMAL MODEL CONSTRUCTION TECHNIQUES

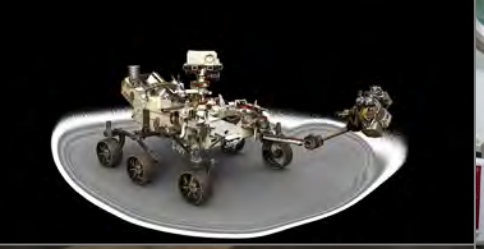
- **The geometries and heat loads are defined in the master file by following the steps listed in the previous slides**
- **Create contactors between the bank geometries and the cell geometries via Domain Tag-sets:**
  - DTS_CELL_TO_FOAM TO DTS_FOAM_TO_CELL
  - DTS_CELL_TO_POS_ENDCAP TO DTS_POS_ENDCAP_TO_CELL
  - 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) $W\ m^{-1}\ °C^{-1}$
  - Prismatic Cell: 28 (x, y) / 3 (z – i.e. thickness) $W\ m^{-1}\ °C^{-1}$
- **Define the convection and radiation environment:**
  - Note that any TD Direct or XREF surface involved with the environment requires the definition of Domain Tag-sets for the interactive surfaces

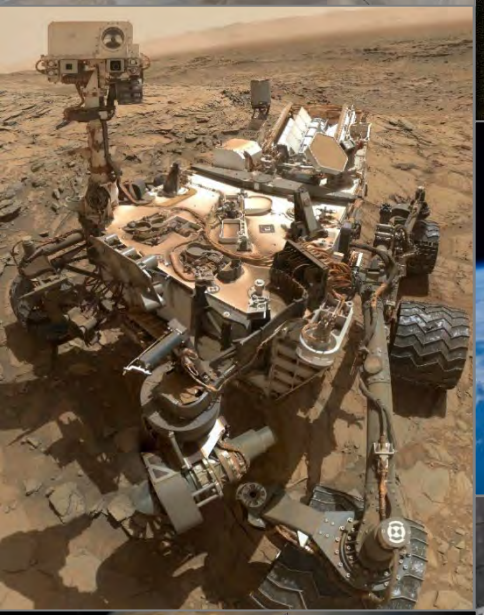


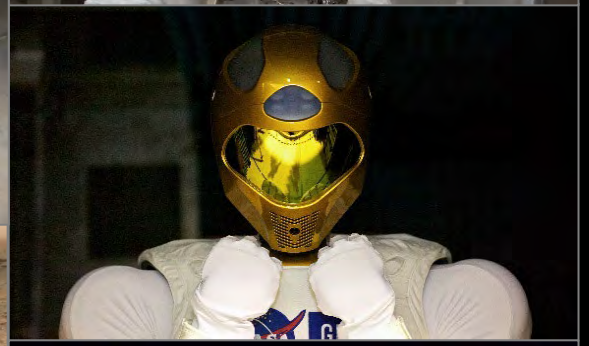
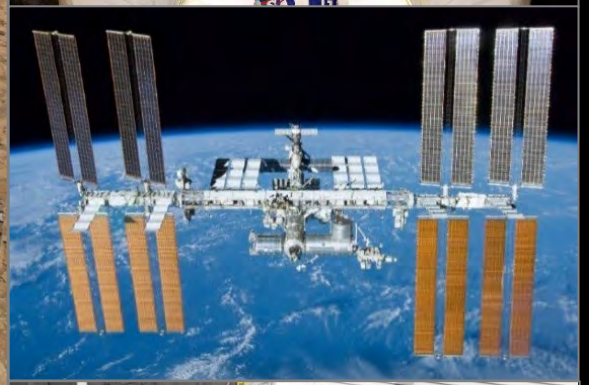
PRACTICAL THERMAL MODEL CONSTRUCTION TECHNIQUES

- **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 tag-sets:**
  - 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 interstitia materials
  - Inside surfaces of endcaps and interstitial materials that will be in contact with th 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**








MODULE 3 SECTION 2:
EXAMPLE THERMAL SIMULATIONS PART 1, NOMINAL OPERATIONS

EXAMPLE OF HEAT GENERATION FROM ELECTROCHEMICAL PROCESSES FOR DISCHARGE

- **Discharge example for a large format 185 Ah $LiCoO_2$ electric vehicle battery based on Chen et. al. [19] and Walker et. al. [20] which compared test and analysis for various discharge rates and convective cooling environment combinations**

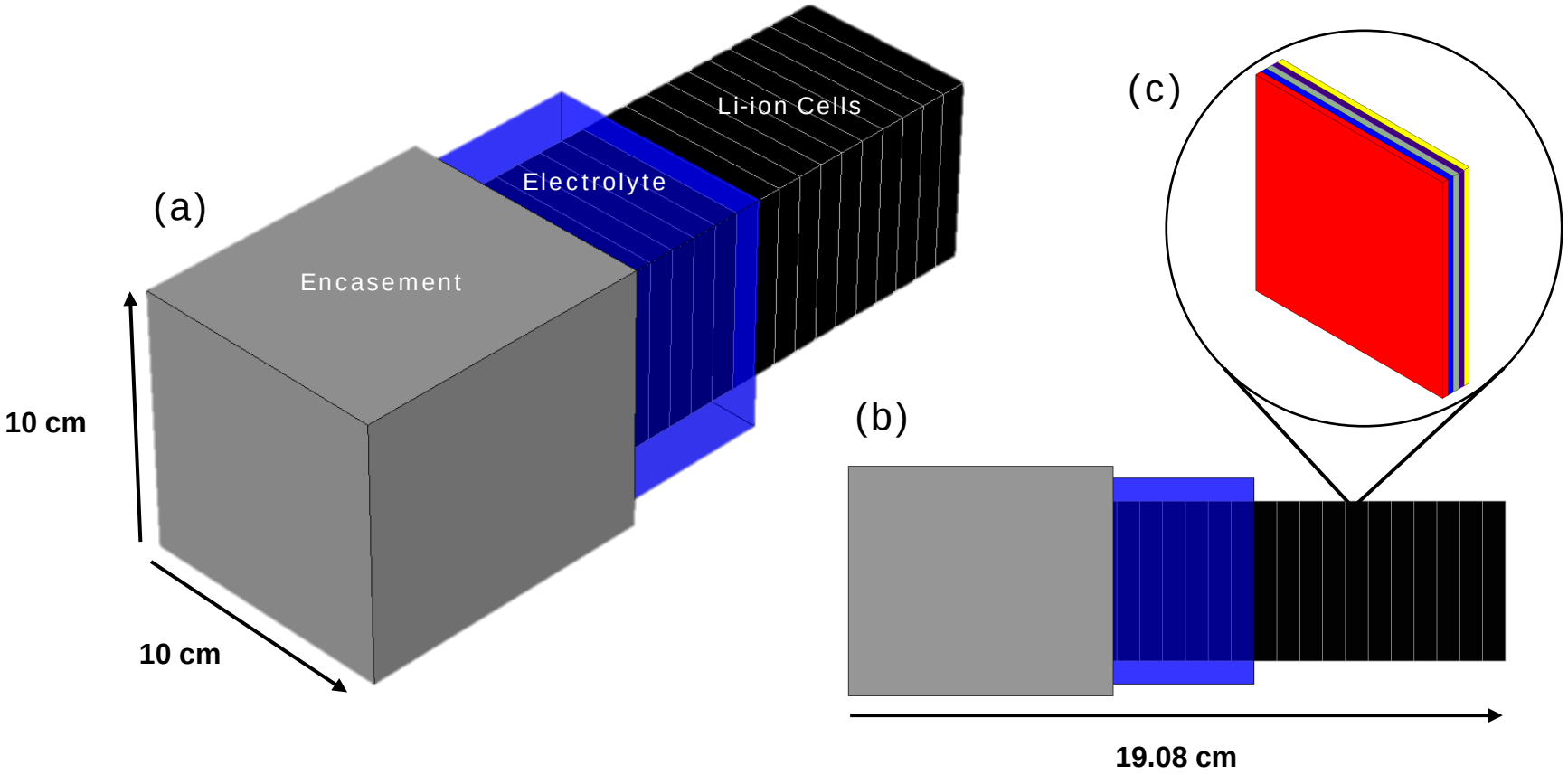
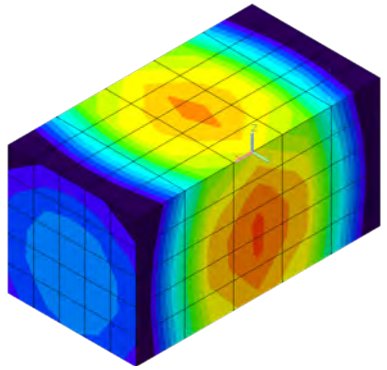


Image courtesy of Walker and Ardebili [20]

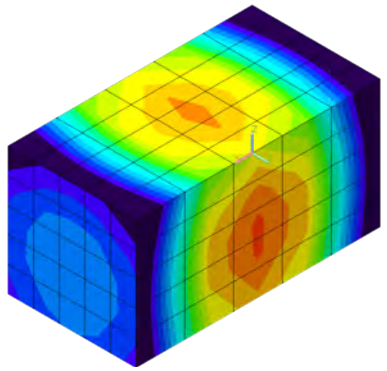
19 S. Chen, C. Wan and Y. Wang, "Thermal Analysis of Lithium-Ion Batteries," Journal of Power Sources, vol. 140, pp. 111-124, September 2005.
20 W. Walker and H. Ardebili, "Thermo-electrochemical analysis of lithium ion batteries for space applications using Thermal Desktop," Journal of Power Sources, vol. 269, pp. 486-497, 2014.

PRACTICAL SIMULATION TECHNIQUES PART 1, NOMINAL OPERATIONS



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

PRACTICAL SIMULATION TECHNIQUES PART 1, NOMINAL OPERATIONS



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

EXAMPLE OF HEAT GENERATION FROM ELECTROCHEMICAL PROCESSES FOR CHARGE

- **Charge example based on various charging rates of a Boston Power Swing 5300 Li-ion cell [21] and Yayathi et. al. [22] :**
  - Note that this example does not employee constant current like the discharge example (see current profile on bottom left image)

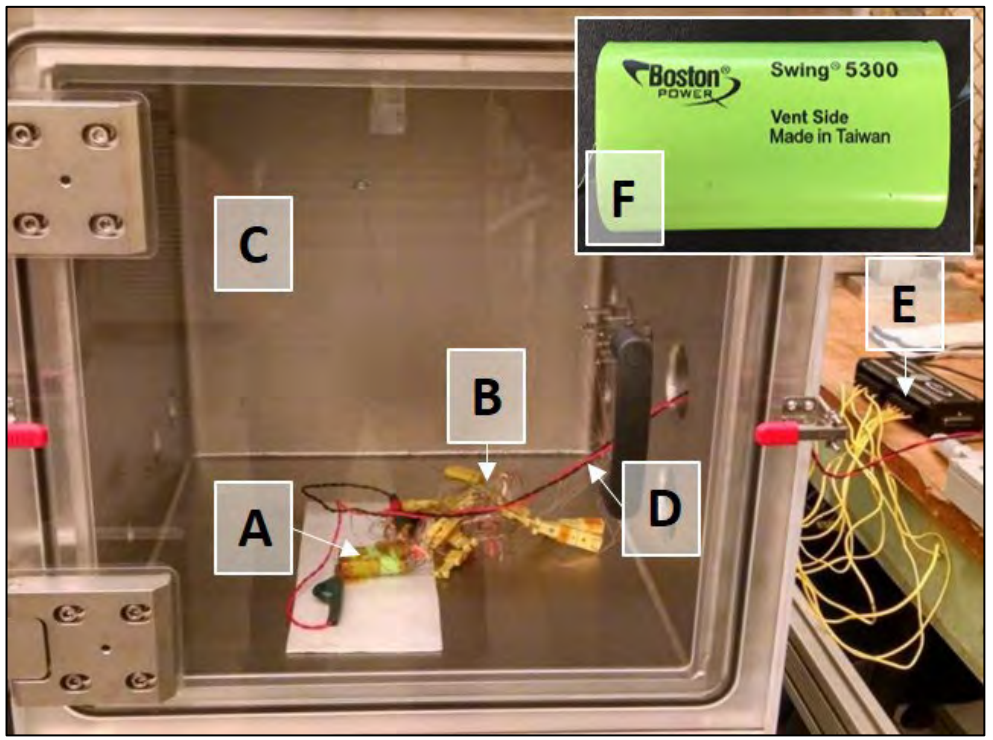
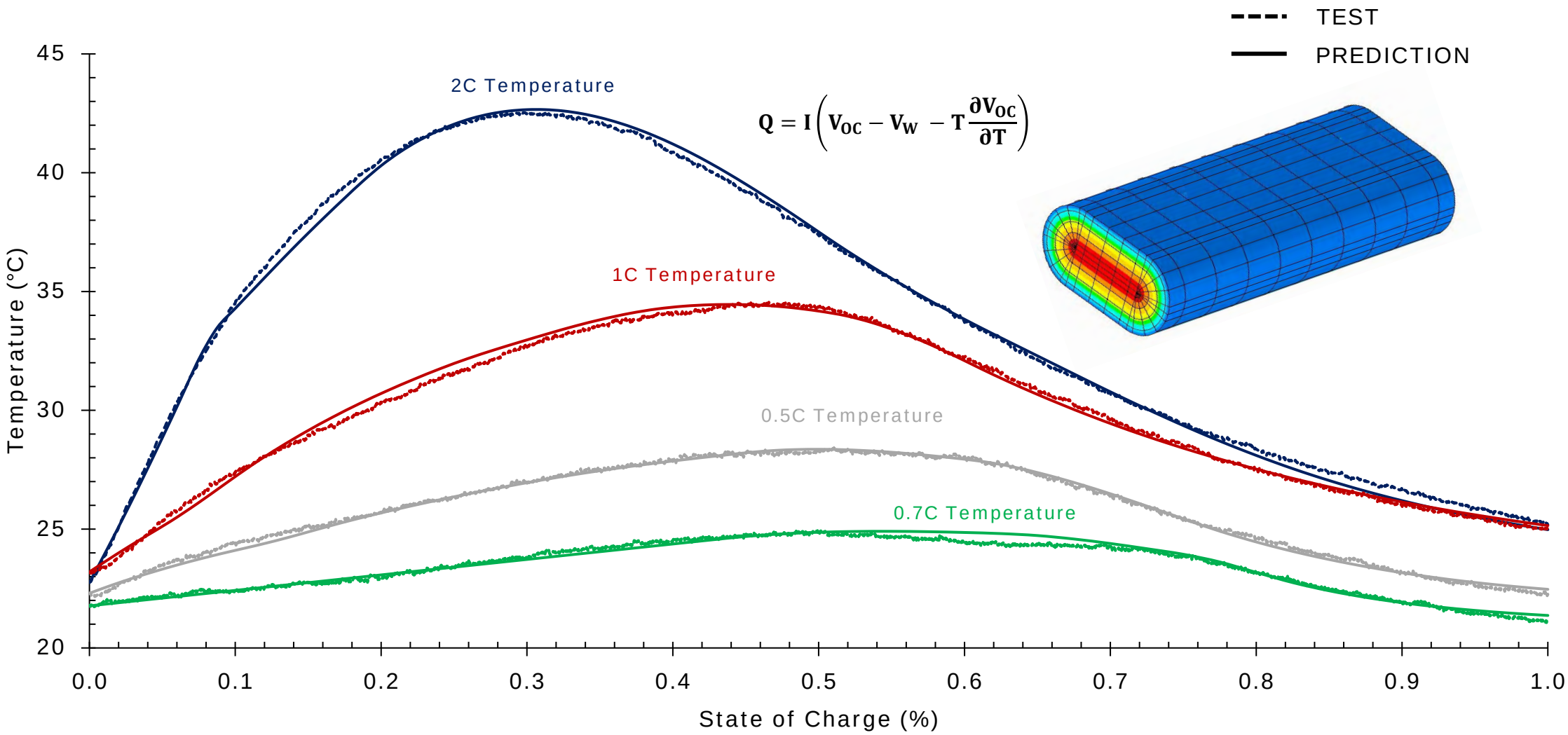


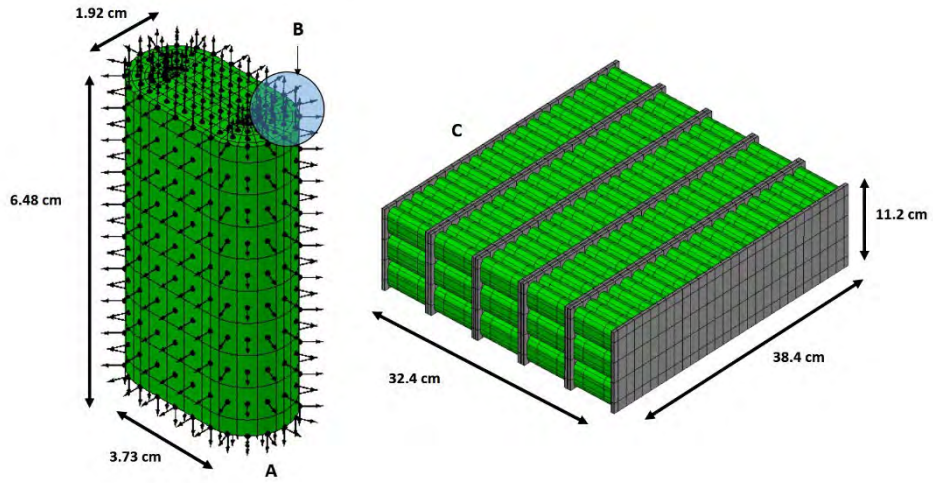
Image courtesy of Walker et. al. [22]

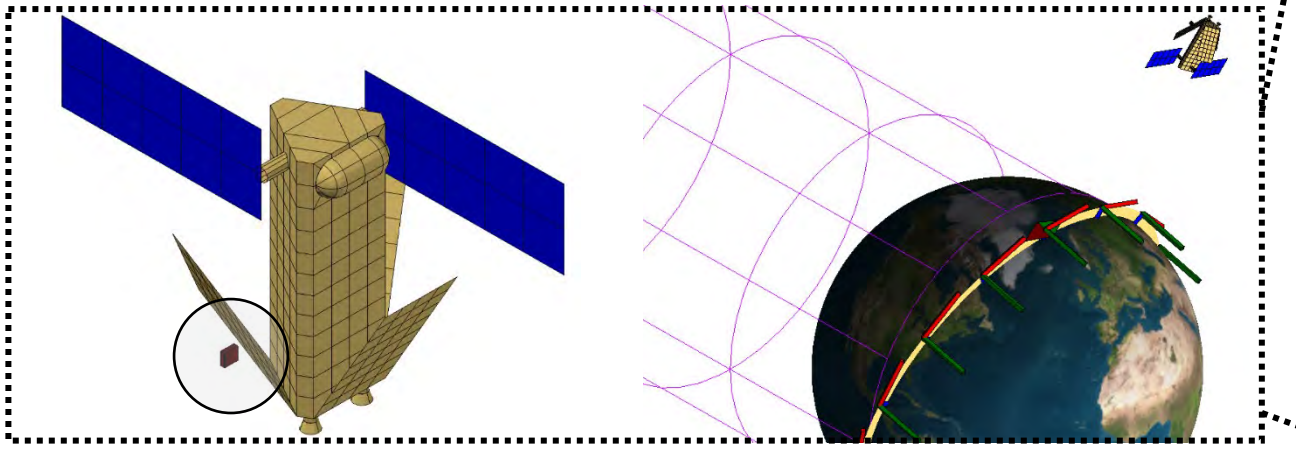
21 Boston Power, *Swing 5300 Rechargeable Lithium-ion Cell*, Westborough: Boston-Power, Incorporated, 2013.
22 W. Walker, S. Yayathi, J. Shaw and H. Ardebili, "Thermo-electrochemical evaluation of lithium-ion batteries for space applications." Submitted to Journal of Power Sources June 27th, 2015.

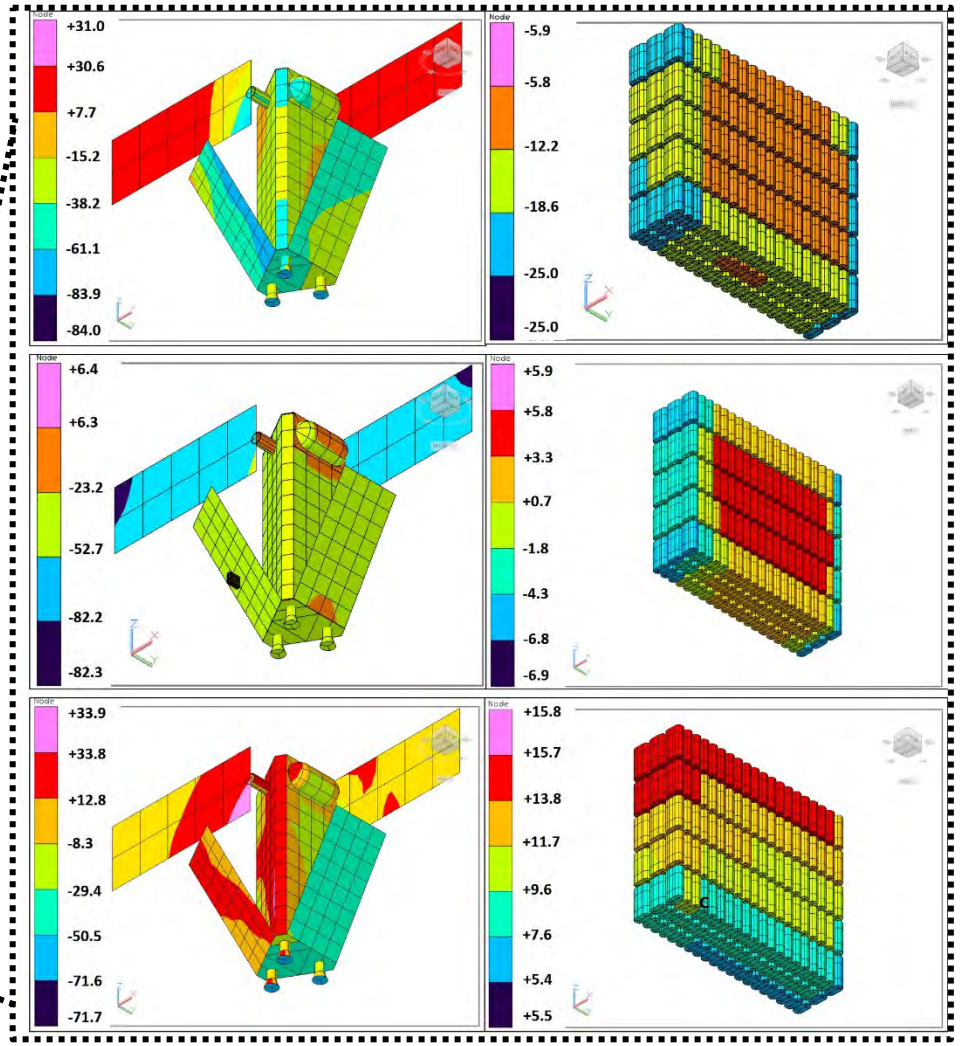
PRACTICAL SIMULATION TECHNIQUES PART 1, NOMINAL OPERATIONS

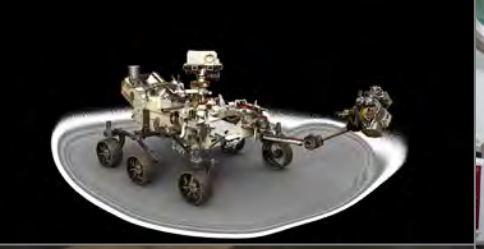


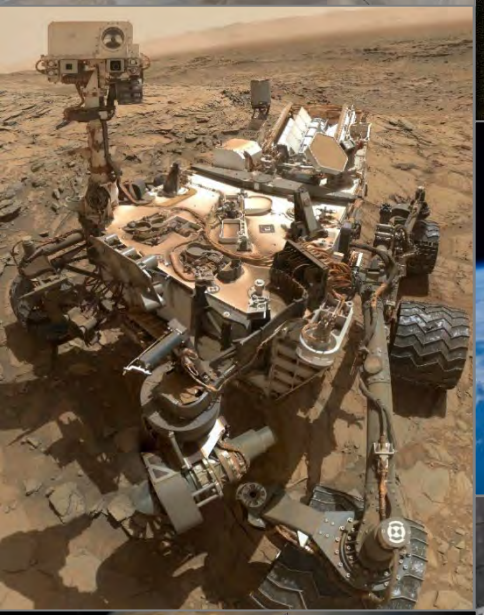
PRACTICAL SIMULATION TECHNIQUES PART 1, NOMINAL OPERATIONS

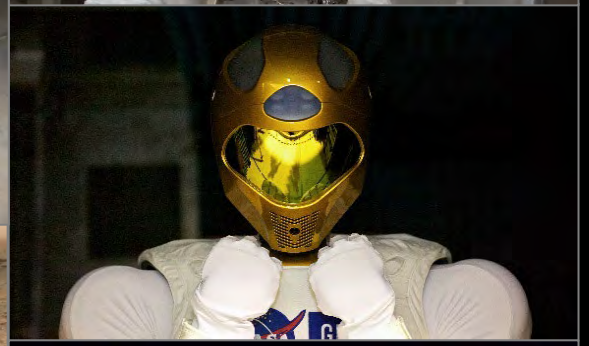
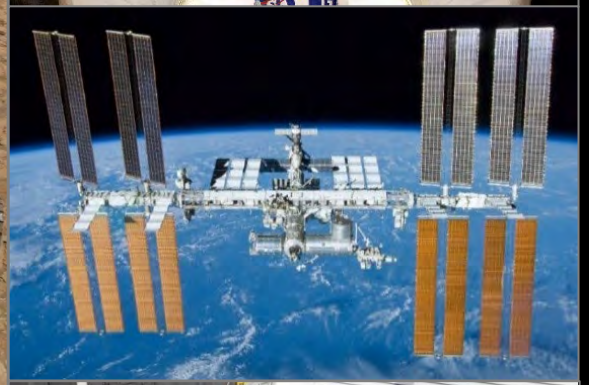











MODULE 3 SECTION 3:
EXAMPLE THERMAL SIMULATIONS PART 2, THERMAL RUNAWAY

DIRECT SIMULATION OF THERMAL RUNAWAY KINETIC RELATIONSHIPS

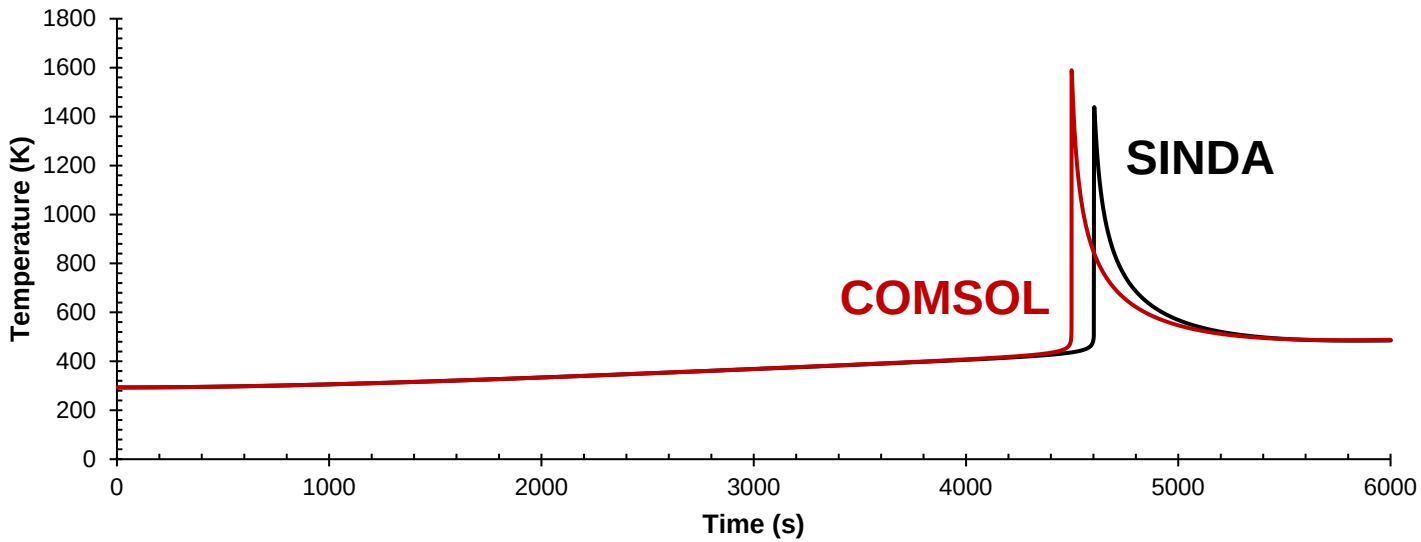
- **Using the previously defined partial differential equations, it is possible to simulate the thermal runaway heat load as a direct function of thermal runaway kinetic relationships:**
  - Examples below compare this method using both COMSOL and SINDA
  - Primary draw-back is that this method is computationally intensive for 0-D simulation, expanding to 3-D only make it more expensive
  - Solution is heavily time-step dependent due to the Arrhenius behavior; large time steps result in inaccurate calculation, small time steps can take too much time to solve
  - Two codes using the same input parameters can result in different answers depending on solver settings (see COMSOL / SINDA comparison)
  - Although helpful in understanding thermal runaway, direct simulation of thermal runaway kinetics is not practical for assembly level simulation

```
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
```

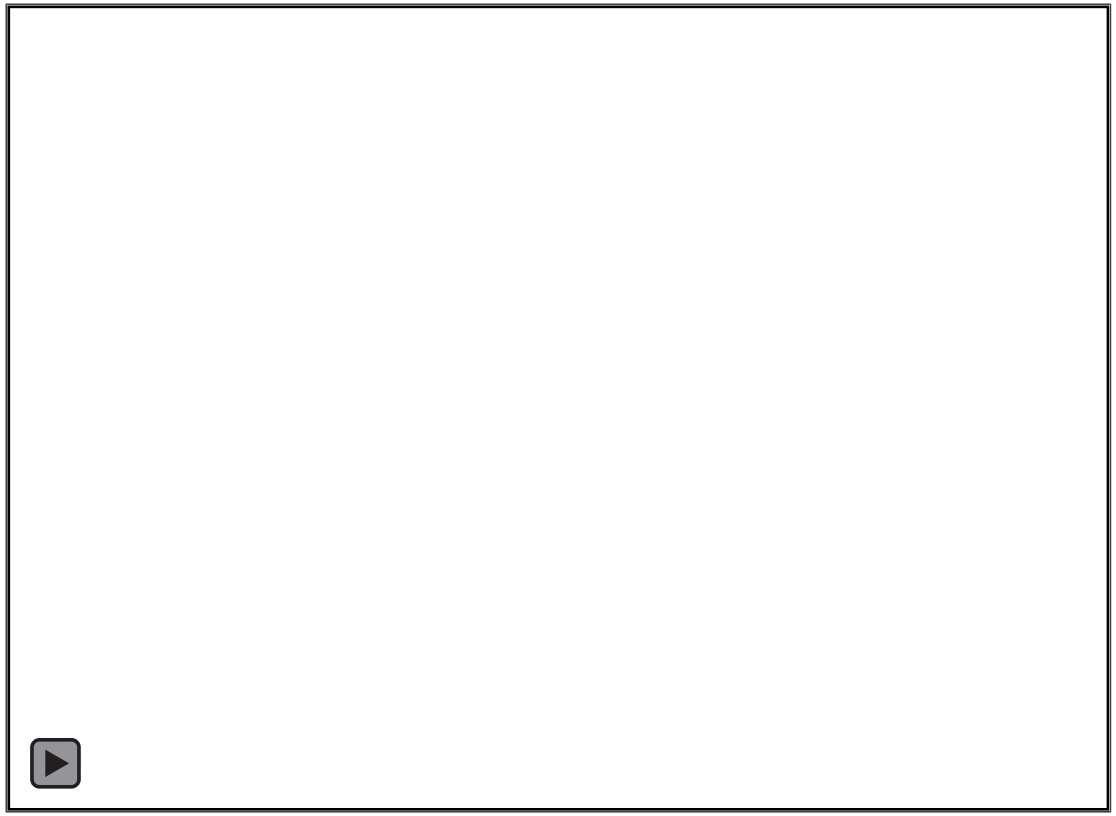


Simulations of environmentally induced thermal runaway based on mathematic models developed by Richard and Dahn, Hatchard et. al., Kim et. al. and Coman et. al. [67-70].

23 Richard, M. Accelerating rate calorimetry study on the thermal stability of lithium intercalated graphite in electrolyte. I. experimental. *Journal of The Electrochemical Society* **146,** 2068 (1999).
24 Hatchard, T., MacNeil, D., Basu, A. & Dahn, J. Thermal model of cylindrical and prismatic lithium-ion cells. *Journal of The Electrochemical Society* **148,** A755 (2001).
25 Kim, G.-H., Pesaran, A. & Spotnitz, R. A three-dimensional thermal abuse model for lithium-ion cells. *Journal of Power Sources* **170,** 476–489 (2007).
26 Coman, P., Rayman, S. & White, R. A lumped model of venting during thermal runaway in a cylindrical Lithium Cobalt Oxide lithium-ion cell. *J Power Sources* **307,** 56–62 (2016).

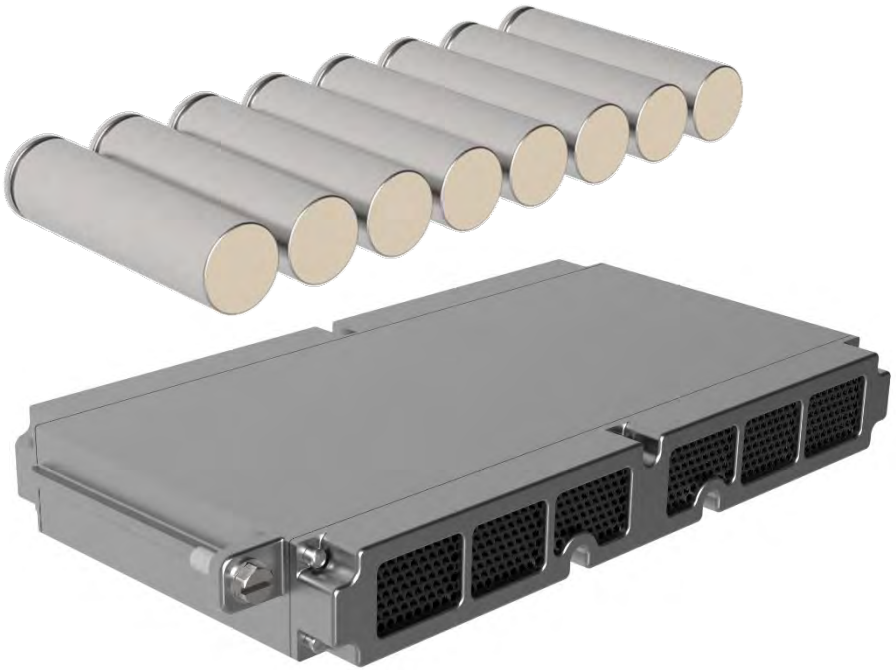
PRACTICAL SIMULATION OF THERMAL RUNAWAY HEATING

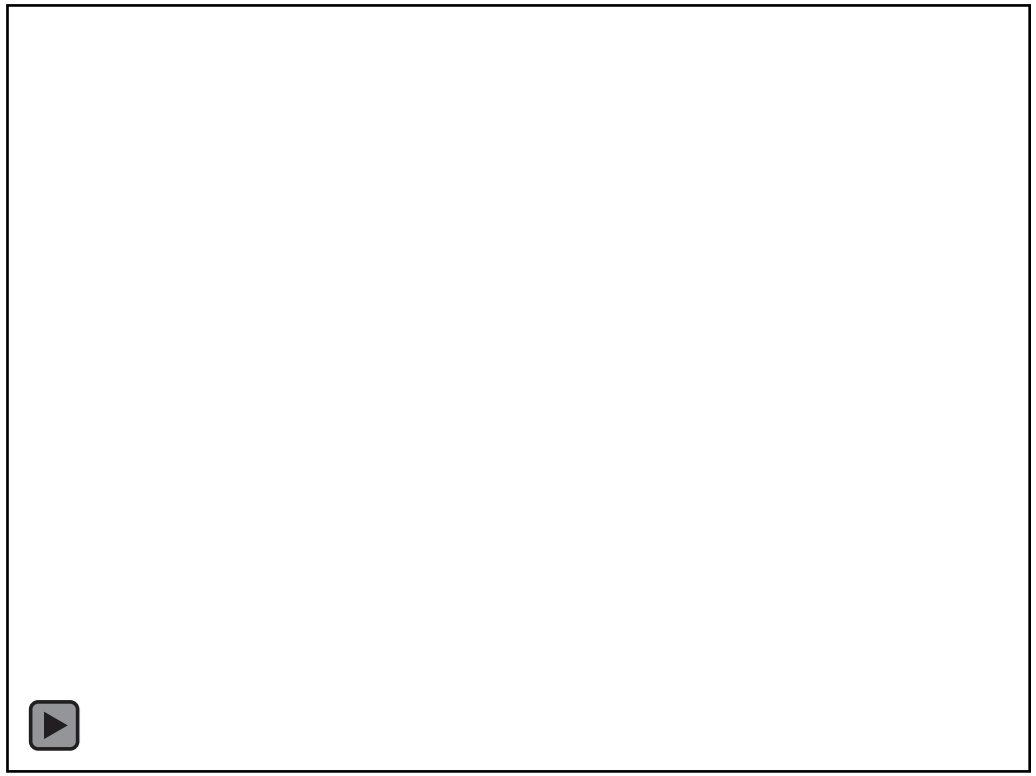
- **Using variable controlled heat loads based on test defined thermal runaway data (i.e. FTRC), it is possible to replicate thermal runaway heating with practical simulation techniques:**
  - The code is designed to do the following at each time step: (1) identify temperatures, (2) observe is thermal runaway criteria is met, (3) continue if not, and (4) apply thermal runaway heat loads when criteria is met
  - Code should have mechanism to ensure that runaway heating only happens once per cell



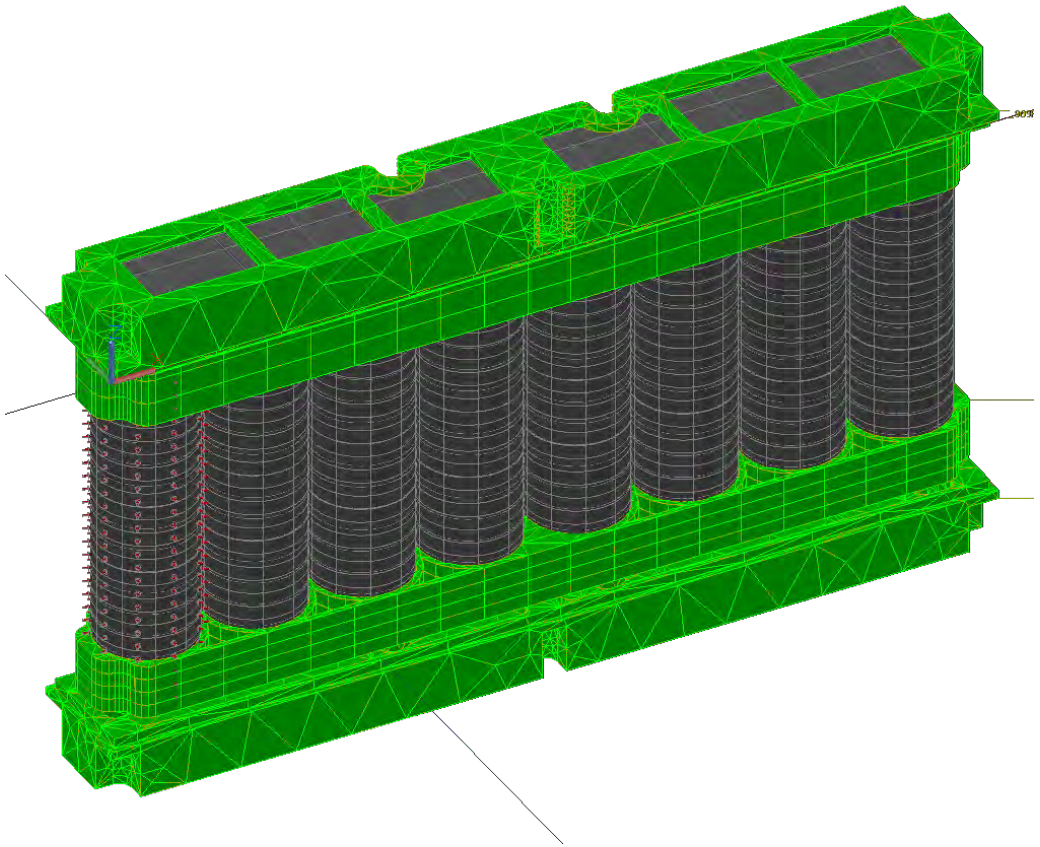
EXAMPLE TEST-CORRELATED THERMAL RUNAWAY ANALYSIS

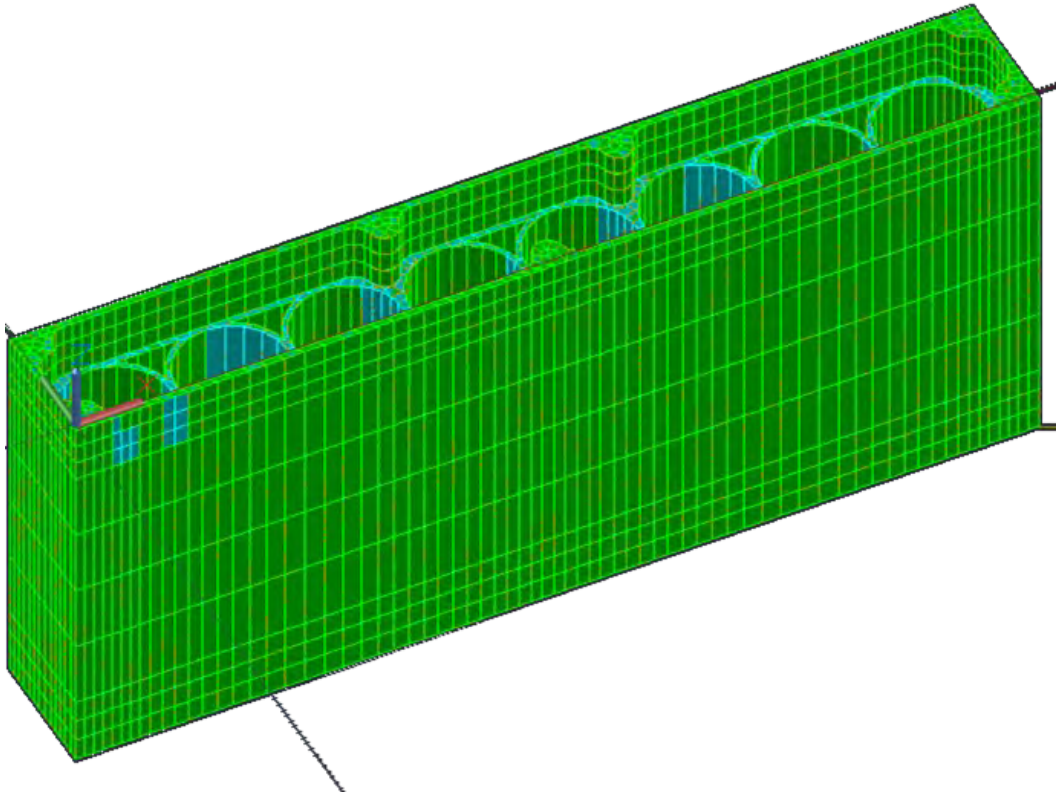
- **Example of test-correlated thermal analysis for abuse testing of a proposed battery assembly for the Advanced Portable Life Support System (PLSS):**
  - Eight 18650 cells encased in an interstitial aluminum housing
  - Challenge is to properly simulate the thermal runaway energy distribution throughout the case
  - The subsequent analysis results are a SNEAK PEAK for an upcoming lecture that provides a detailed discussion on practical simulation of thermal runaway in battery assemblies





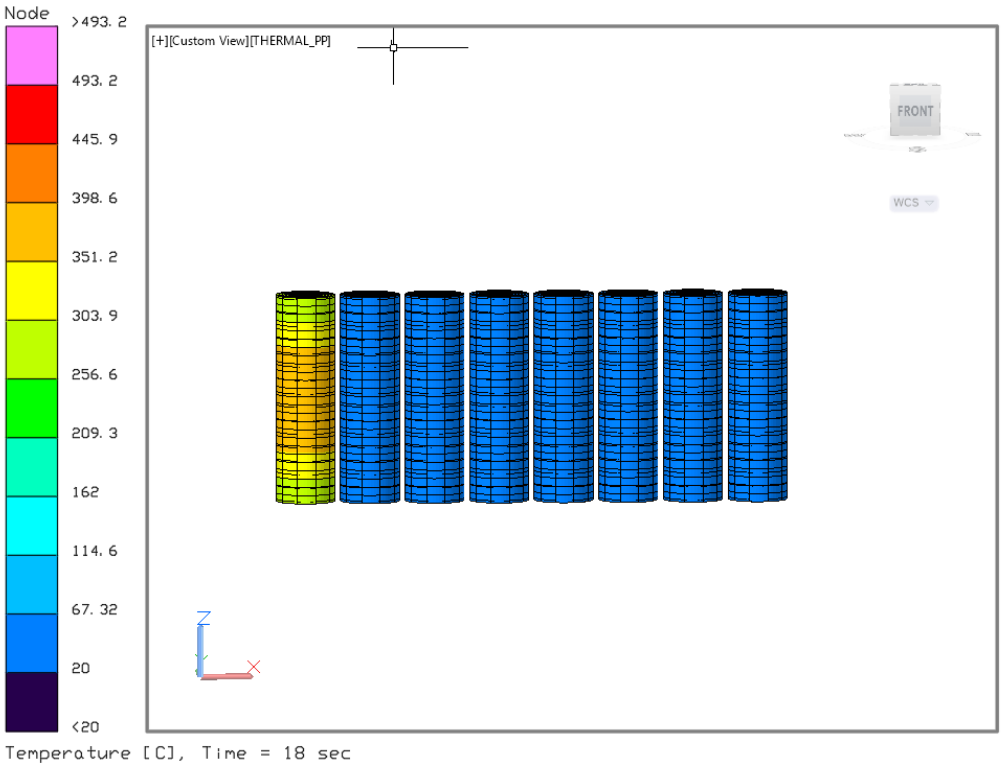
EXAMPLE TEST-CORRELATED THERMAL RUNAWAY ANALYSIS



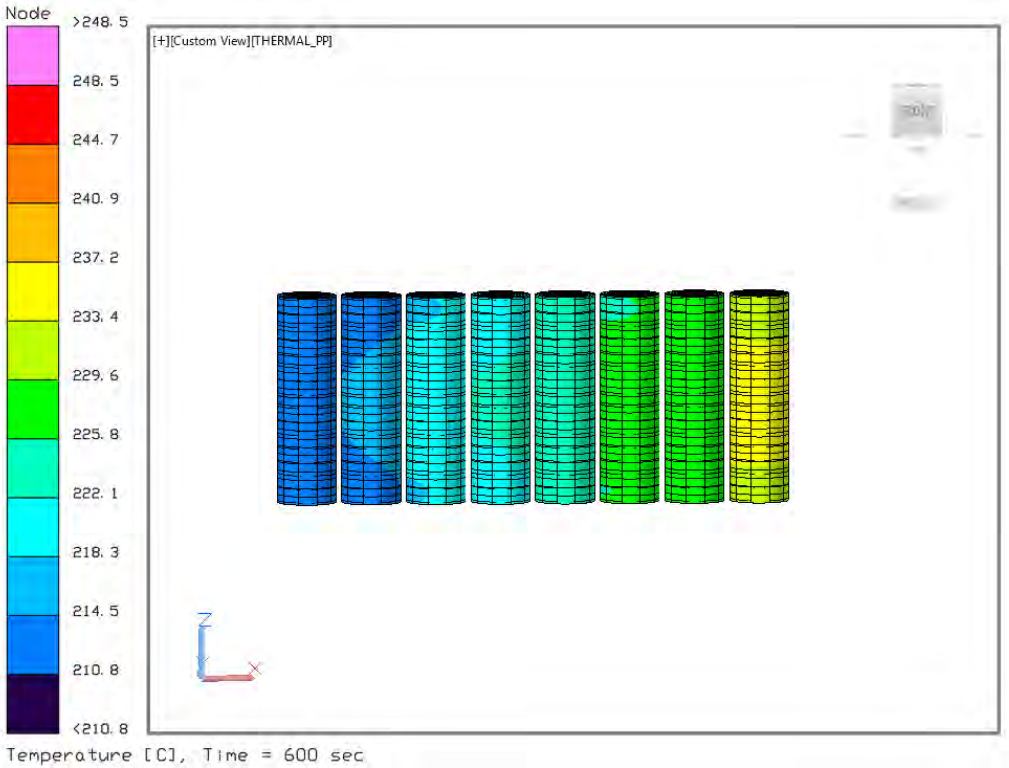


Credit: Stephania Ortega (NASA JSC)

EXAMPLE TEST-CORRELATED THERMAL RUNAWAY ANALYSIS



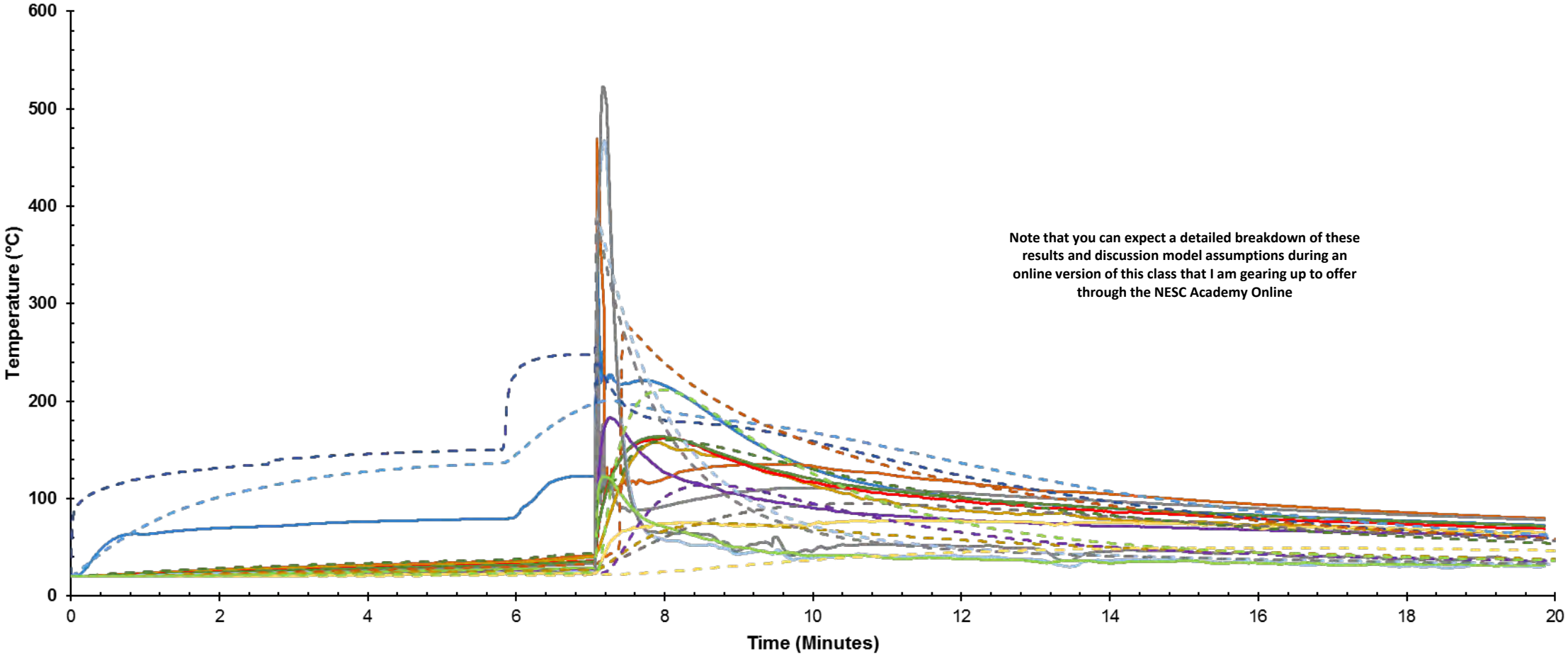
First Cell Temperature Peak



End of Transient Simulation

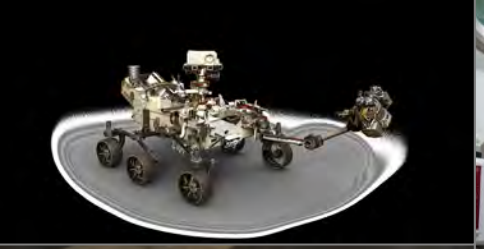
Credit: Stephania Ortega (NASA JSC)

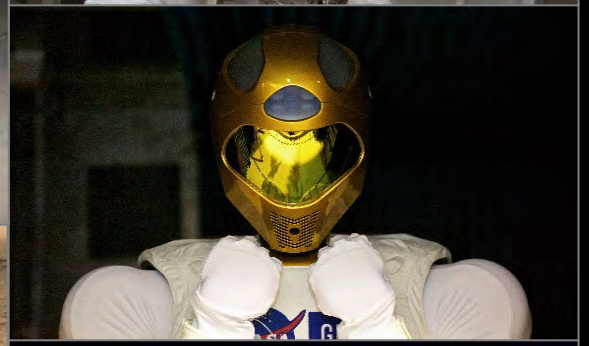
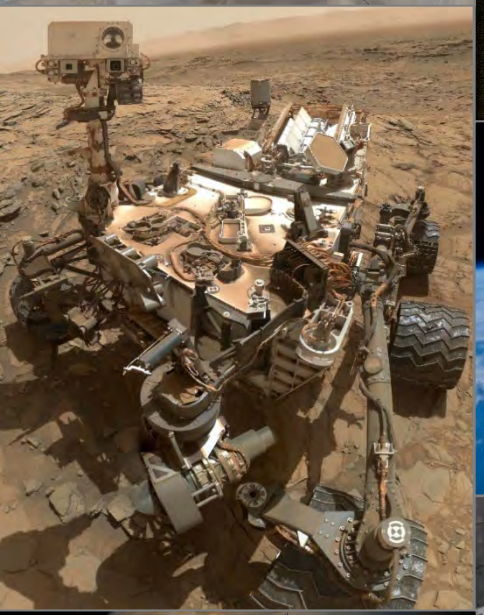
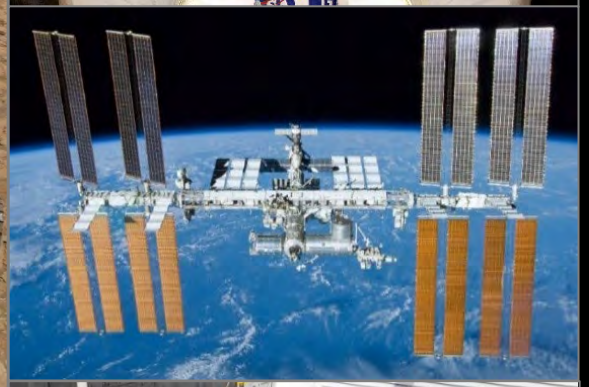
EXAMPLE TEST-CORRELATED THERMAL RUNAWAY ANALYSIS



Note that you can expect a detailed breakdown of these results and discussion model assumptions during an online version of this class that I am gearing up to offer through the NESC Academy Online

Credit: Stephania Ortega (NASA JSC)



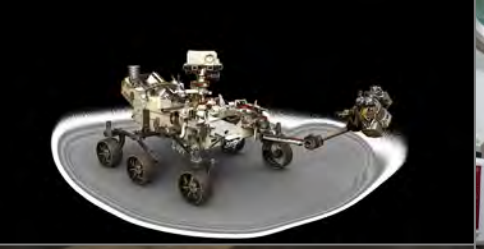





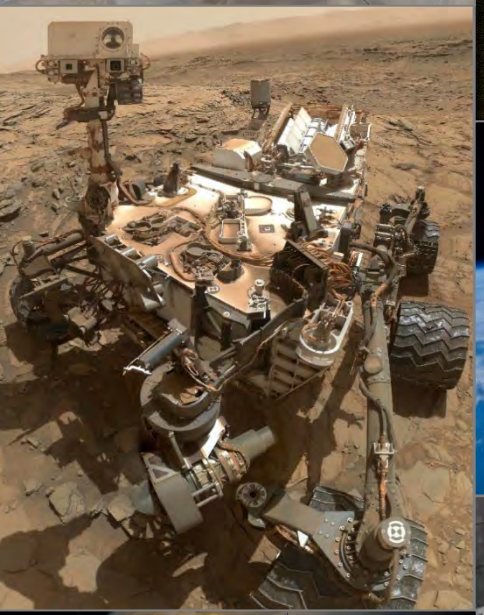


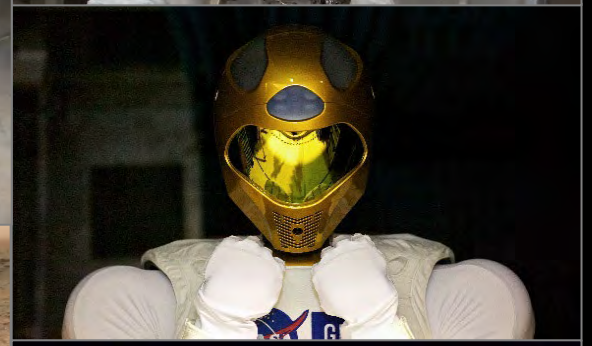
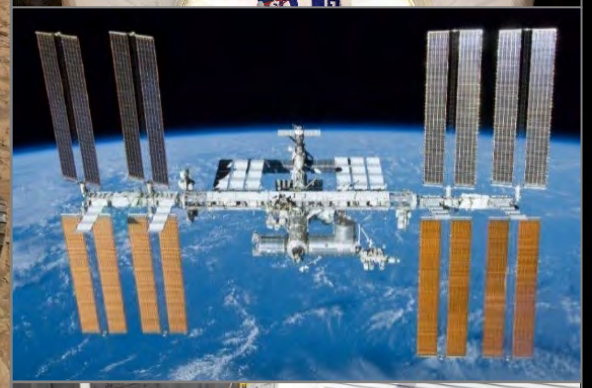
WRAP-UP AND QUESTIONS

ACKNOWLEDGEMENTS

- NASA Engineering and Safety Center
- NASA JSC Engineering Directorate (EA), Structural Engineering Division (ES) and Power and Propulsion Division (EP)
- Steve Rickman, Eric Darcy, and Christopher Iannello
- NASA JSC Energy Systems Test Area (ESTA)
- Haleh Ardebili






QUESTIONS?