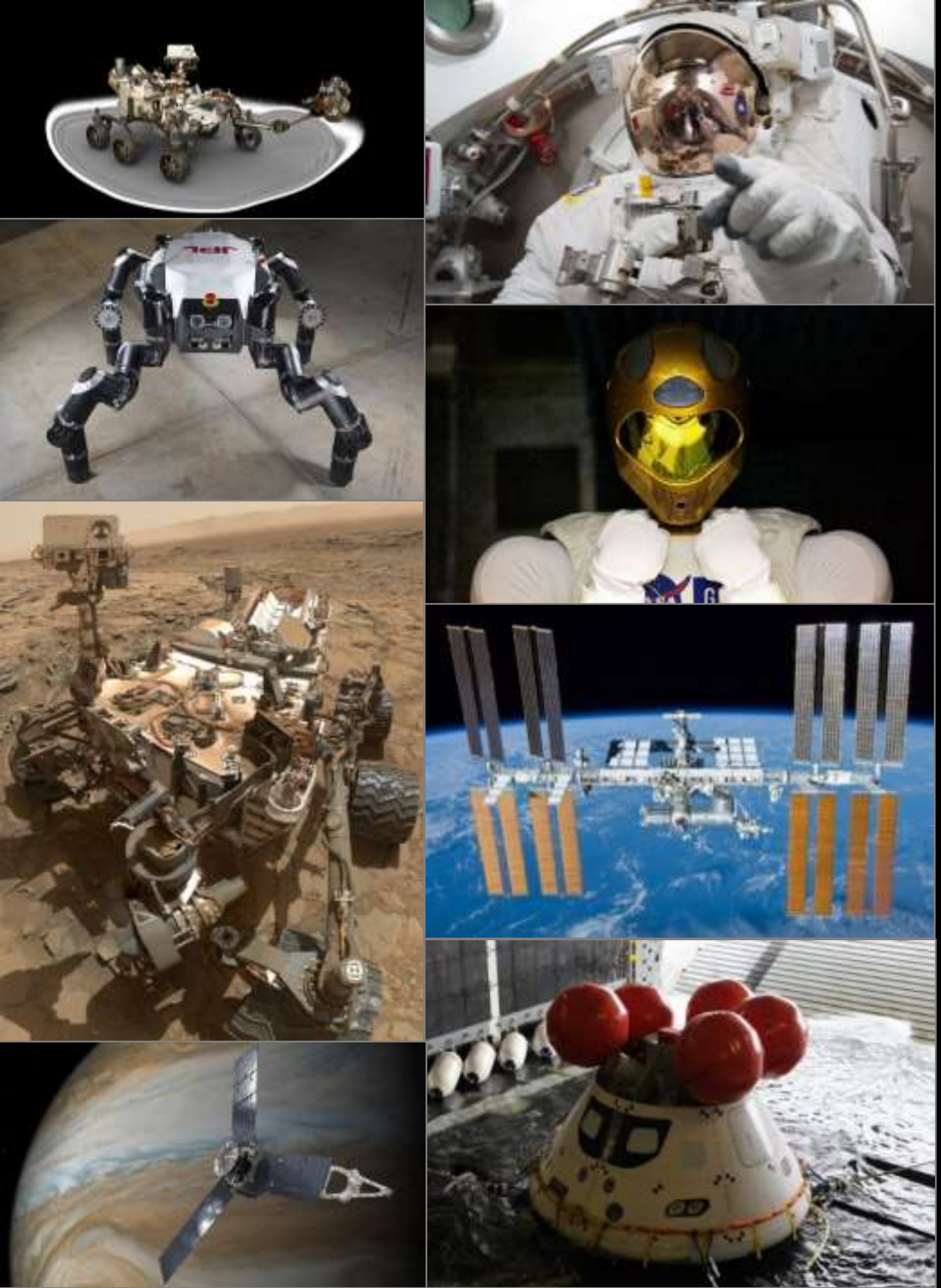


COMBINING FRACTIONAL CALORIMETRY WITH STATISTICAL METHODS TO CHARACTERIZE THERMAL RUNAWAY

William Walker, Ph.D. [1,2]
william.walker@nasa.gov

Additional Contributors: John Darst [1,2], Donal Finegan, Ph.D. [3], Peter J. Hughes [1,2,4], Saul Pizano [1,2,4], Eric Darcy, Ph.D. [1,2]

Advanced Automotive Battery Conference
May 24th-25th, 2019
San Diego, California

[1] *National Aeronautics and Space Administration (NASA)*
[2] *Johnson Space Center (JSC)*
[3] *National Renewable Energy Laboratory (NREL)*
[4] *University Space Research Association (USRA)*

NASA STRATEGY TO PROTECT AGAINST THERMAL RUNAWAY

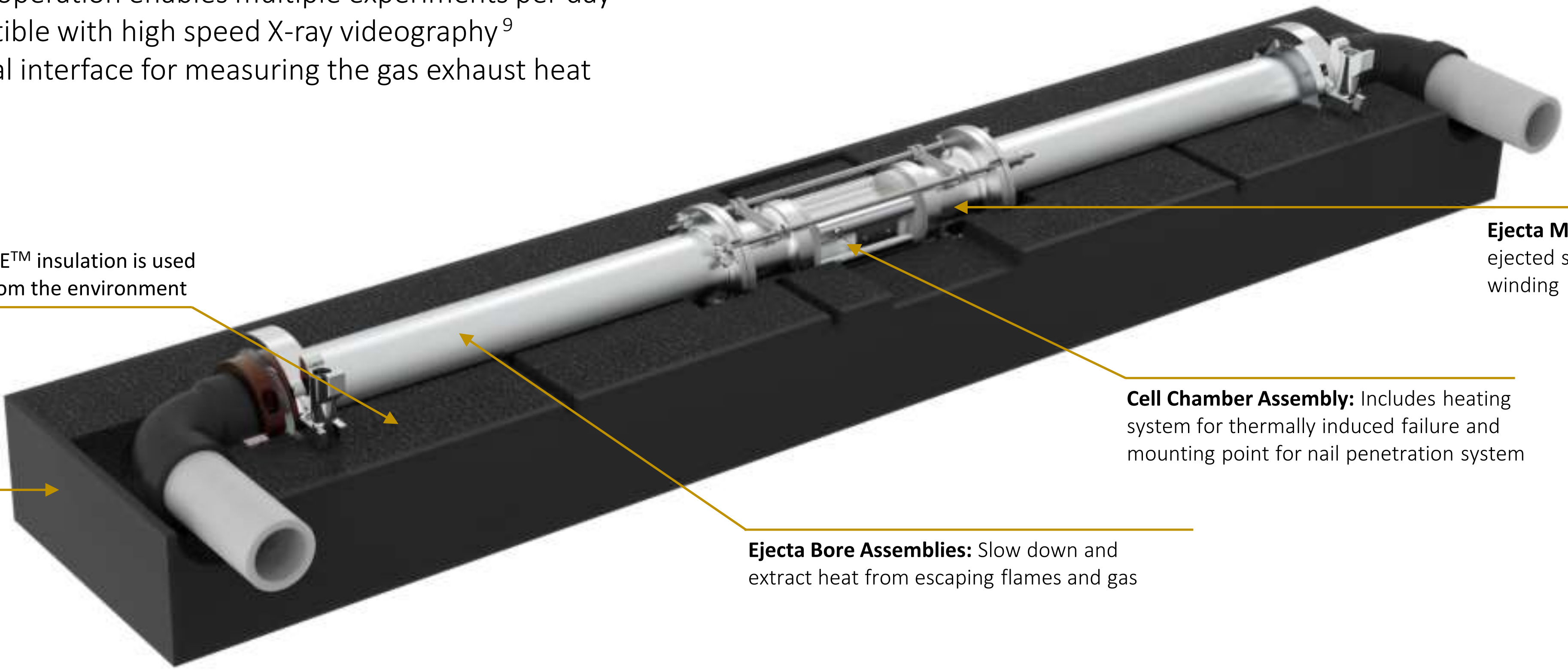
- **Following the 2013 Boeing 787 Dreamliner incident, NASA teams developed new definitions for battery design success criteria:**
  - Always assume thermal runaway (TR) will eventually happen
  - Design should ensure that TR event is not catastrophic
  - Demonstrate that propagation to surrounding cells will not occur
- **Thermal management systems designed to mitigate the effects of thermal runaway and prevent cell-to-cell propagation should consider the following** [1]**:**
  - No two runaway events are 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
- **Optimization of Li-ion battery assemblies that satisfy the aforementioned strategies requires knowledge of the following:**
  - 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

---

[1] *Crewed Space Vehicle Battery Safety Requirements. JSC-20793 Rev D. JSC Engineering Directorate, Power and Propulsion Division*

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



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

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

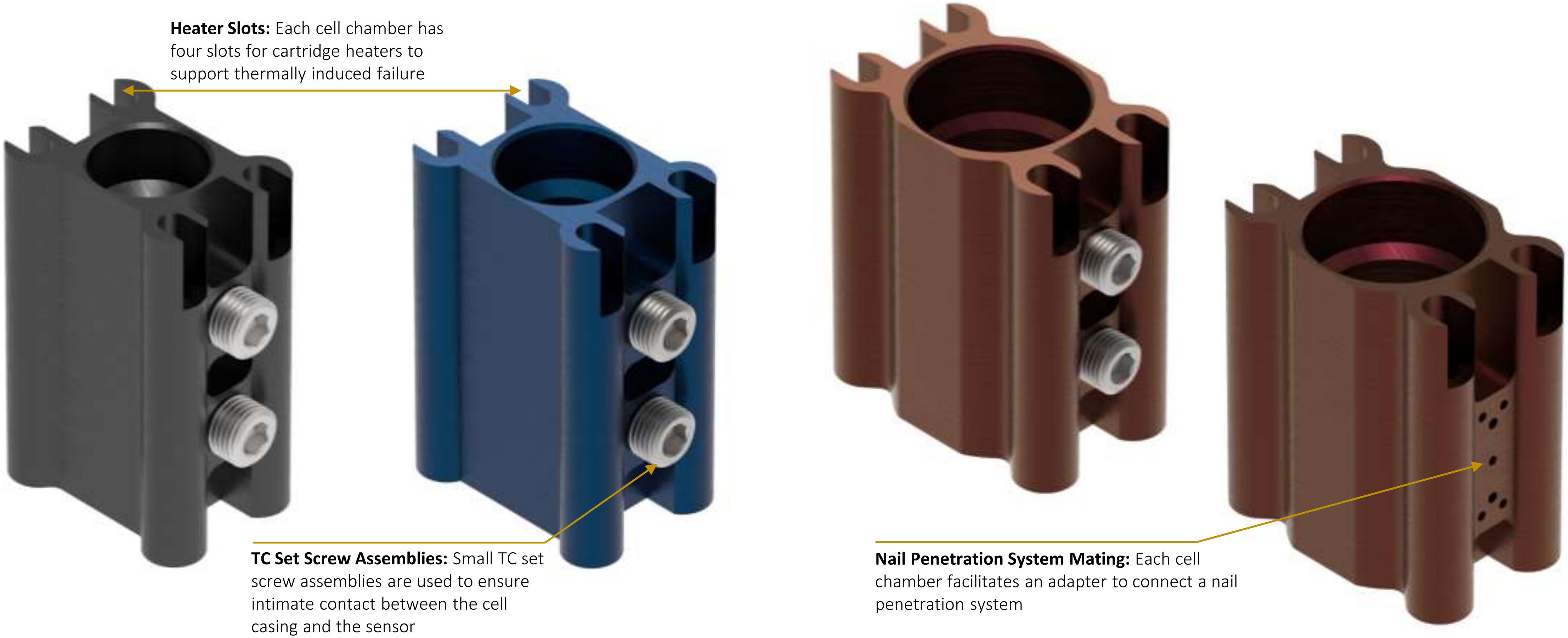
Cell Chamber Assembly: Includes heating system for thermally induced failure and mounting point for nail penetration system

Housing: Lightweight and shipping ready housing is employed to support hardware mobility

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

FRACTIONAL THERMAL RUNAWAY CALORIMETRY

- **The FTRC currently supports cell chambers designed for the following cell formats: 18650, 21700, and D-Cell:**
  - Utilizes the same downstream FTRC assemblies (i.e. the only adjustment to test a new cell is to swap out the cell chamber)
  - The current architecture supports cells with >5 Ah capacities
  - Stay tuned for new capabilities to support pouch cells and larger format cells…



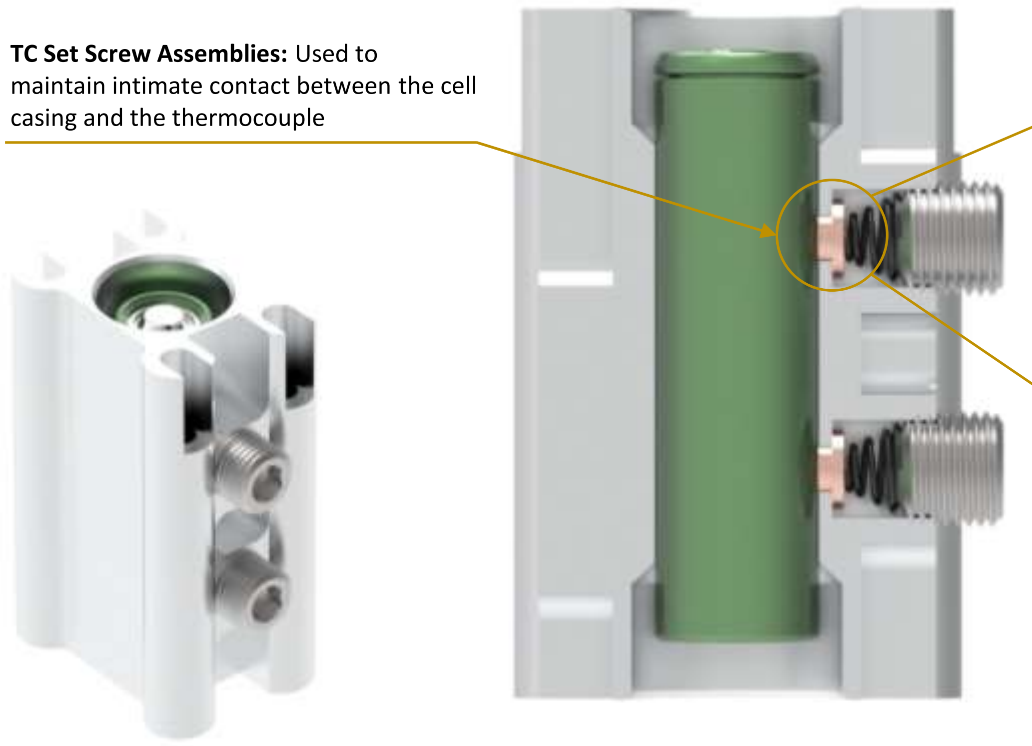
Heater Slots: Each cell chamber has four slots for cartridge heaters to support thermally induced failure

TC Set Screw Assemblies: Small TC set screw assemblies are used to ensure intimate contact between the cell casing and the sensor

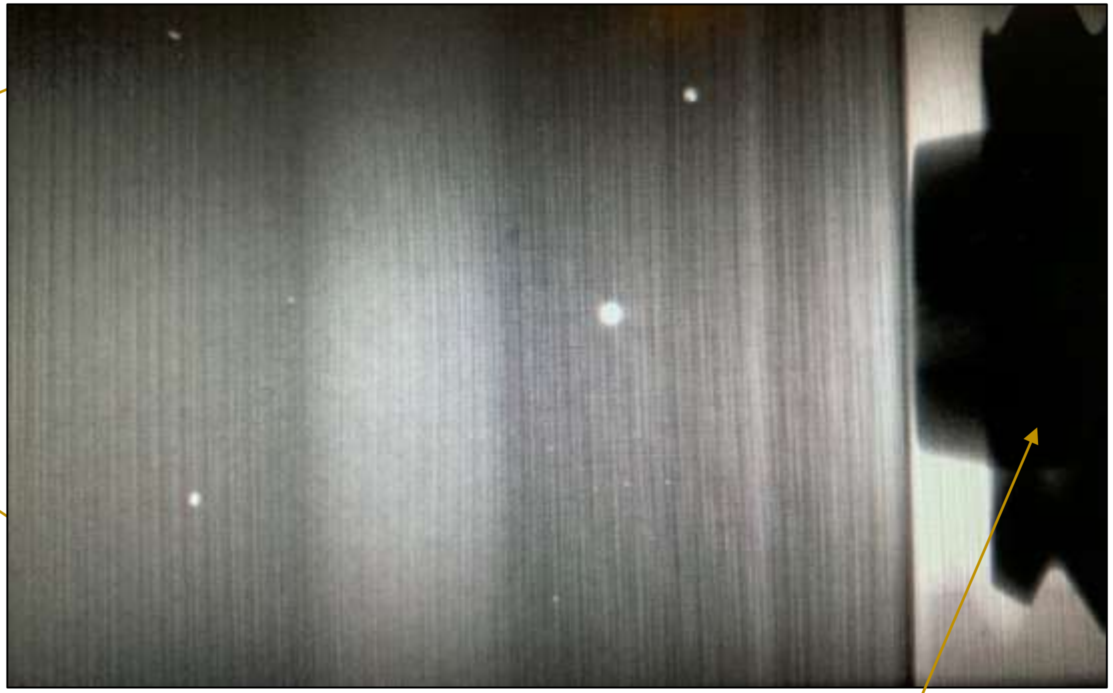
Nail Penetration System Mating: Each cell chamber facilitates an adapter to connect a nail penetration system

FRACTIONAL THERMAL RUNAWAY CALORIMETRY

- **Reliable temperature measurement from the side of the cell is critical to accurate calculation of the fraction of thermal runaway energy released through the cell casing:**
  - To support temperature measurement on the cell casing without actually installing a thermocouple, the FTRC cell chambers employ plunger like set screw assemblies that contain an imbedded thermocouple
  - When released, the spring loaded set screw assembly forces intimate contact between the embedded thermocouple and the cell casing



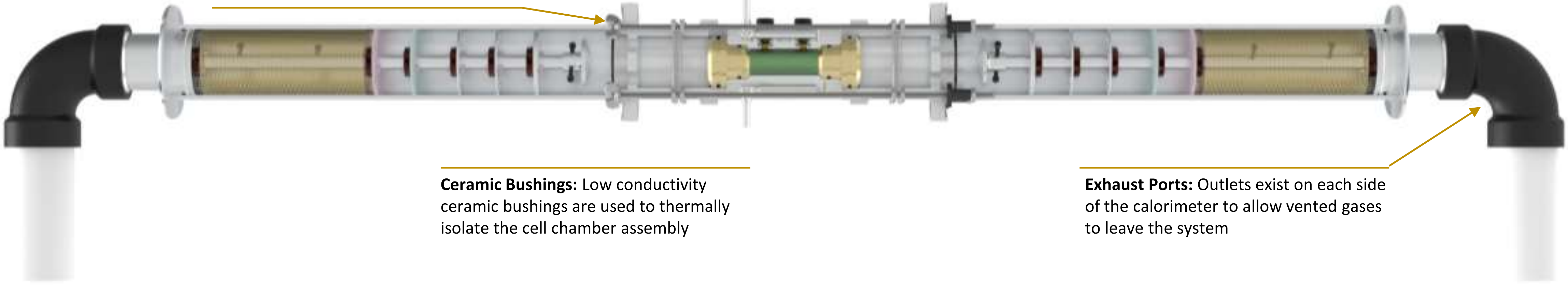
TC Set Screw Assemblies: Used to maintain intimate contact between the cell casing and the thermocouple



X-Ray Image: Image reveals the contact between the TC set screw assembly and an 18650 Li-ion cells installed in the FTRC during testing at Diamond Light Source in 2019.

FRACTIONAL THERMAL RUNAWAY CALORIMETRY

- **The FTRC is designed to not only facilitate testing of different cell types, but to also help characterize directional/fractional thermal runaway failure behavior (i.e. top vent, bottom vent, ruptures from any location, et…)**
- **The cell chamber assembly is isolated from the remainder of the up and down stream calorimeter components with low conductivity ceramic bushings:**
  - Maintaining this thermal isolation is critical to our team's ability to discern the fraction of energy released through the cell casing vs. through the ejecta material
  - The ejecta mating segment is designed to capture and stop complete jellyroll ejections; with this capability, we can also determine the fraction of energy associated with an ejected jellyroll



Symmetric (Ambidextrous) Design: Supports both top and bottom vent (and rupture) thermal runaway behavior

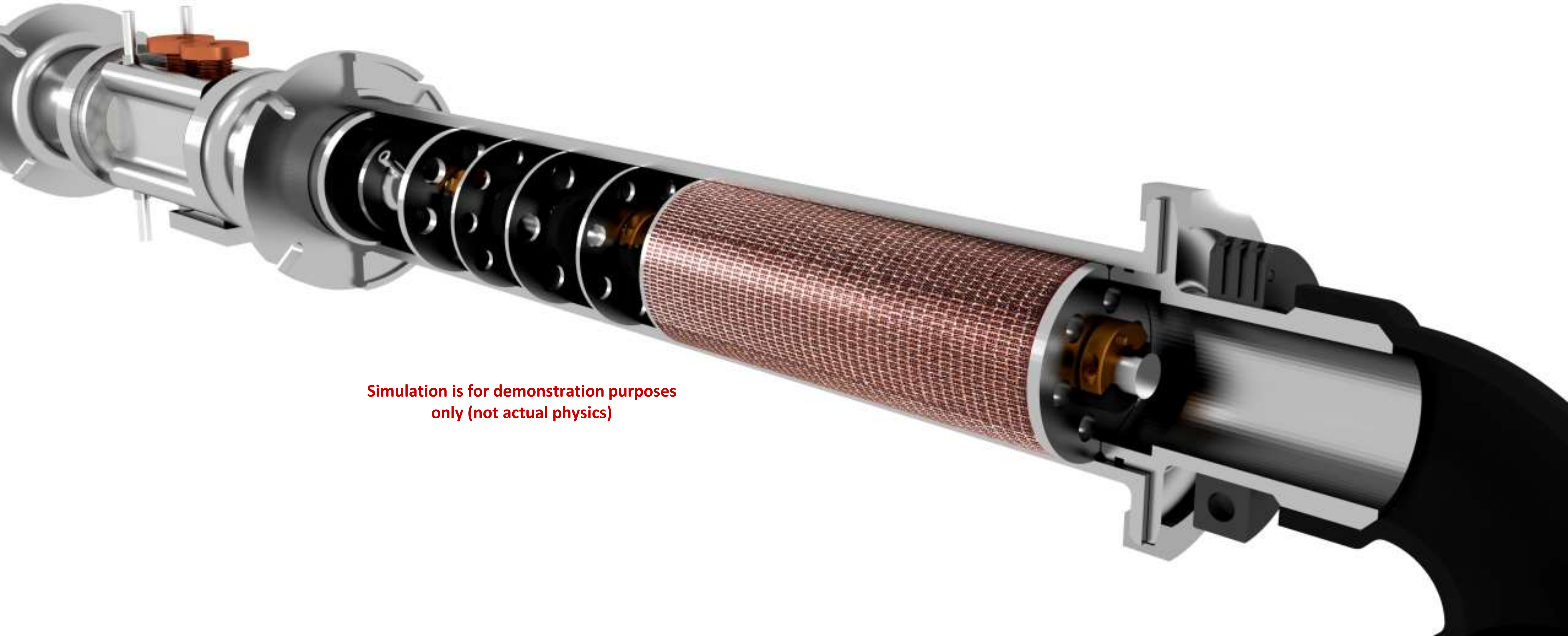
Tie Rods: Spring loaded tie rods are used to clamp the up and down stream components together

Ceramic Bushings: Low conductivity ceramic bushings are used to thermally isolate the cell chamber assembly

Exhaust Ports: Outlets exist on each side of the calorimeter to allow vented gases to leave the system

FRACTIONAL THERMAL RUNAWAY CALORIMETRY

- The internal baffles and copper mesh are used to create a tortuous path that effectively reduces flow velocity, captures large and fine ejected particulates, and cools down the flowing particles and gases before they exit the system (i.e. captures the energy)



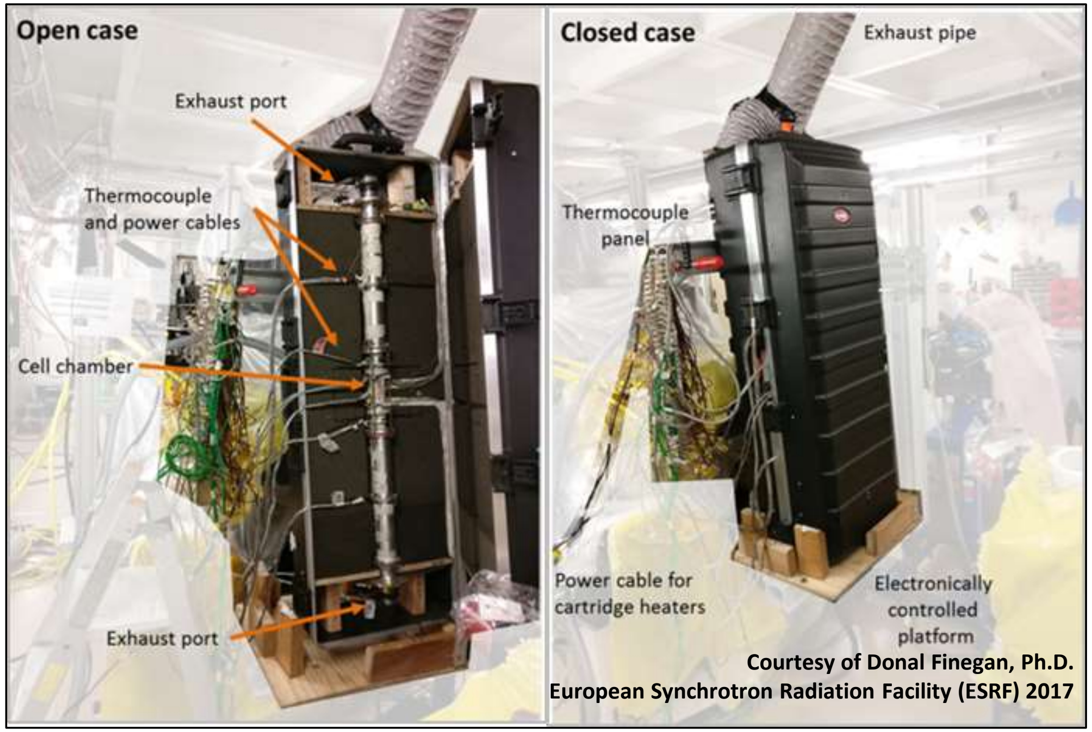
Simulation is for demonstration purposes only (not actual physics)

EXAMPLE FTRC TESTING

NASA Johnson Space Center
Energy Systems Test Area (ESTA)
September 27th, 2018
FTRC: LG 18650-HG2

FRACTIONAL THERMAL RUNAWAY CALORIMETRY

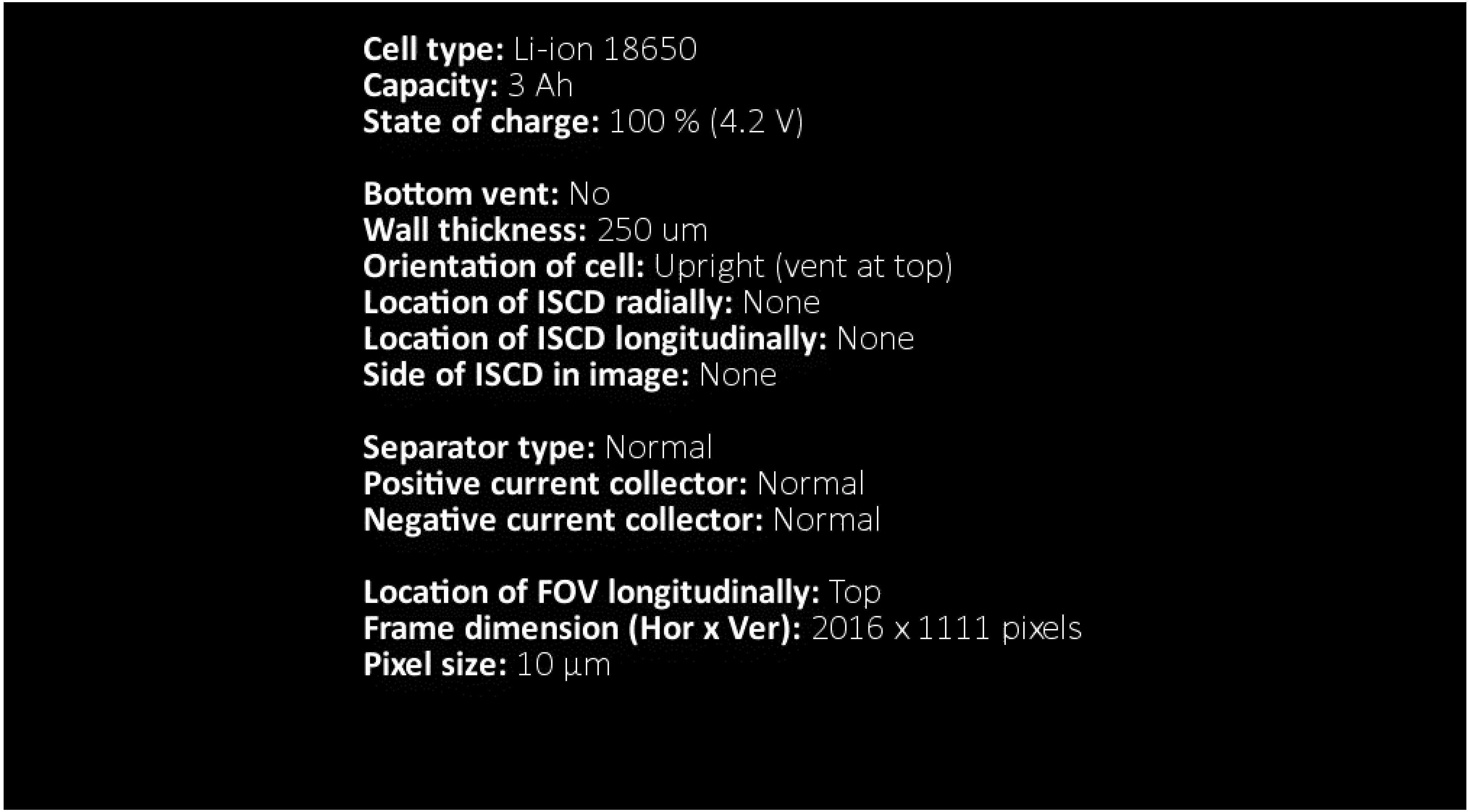
- **Images below depict the global testing capability of the device:**
  - FTRC testing at the NASA JSC Energy Systems Test Area
  - FTRC testing at the European Synchrotron Radiation Facility (ESRF) for in-situ high speed tomography (left image)
  - FTRC testing at the Diamond Light Source (DLS) Facility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



Courtesy of Donal Finegan, Ph.D.
European Synchrotron Radiation Facility (ESRF) 2017

Courtesy of William Walker, Ph.D.
Diamond Light Source (DLS) 2019

HIGH SPEED XRAY VIDEOGRAPHY



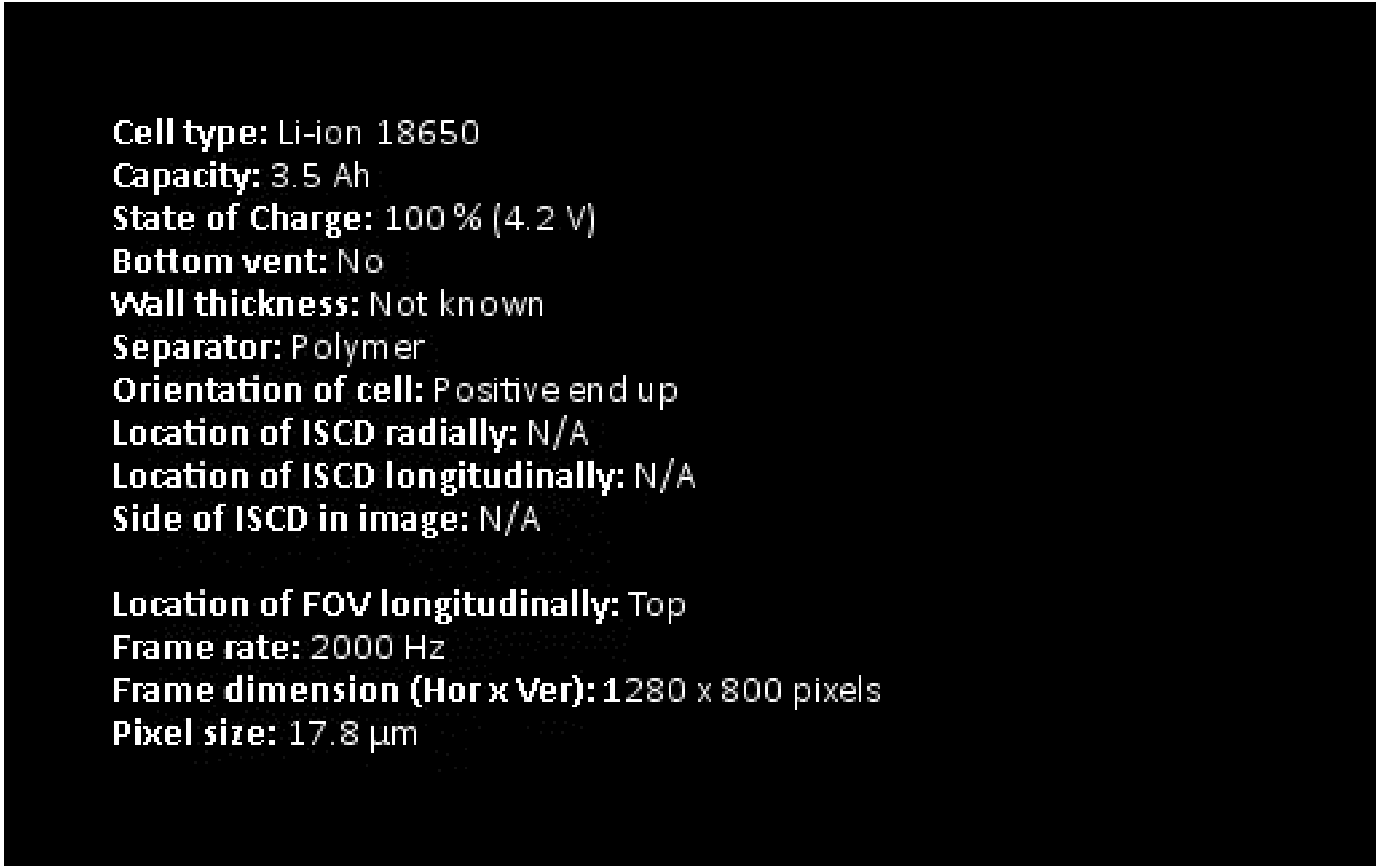
Cell type: Li-ion 18650
Capacity: 3 Ah
State of charge: 100 % (4.2 V)

Bottom vent: No
Wall thickness: 250 um
Orientation of cell: Upright (vent at top)
Location of ISCD radially: None
Location of ISCD longitudinally: None
Side of ISCD in image: None

Separator type: Normal
Positive current collector: Normal
Negative current collector: Normal

Location of FOV longitudinally: Top
Frame dimension (Hor x Ver): 2016 x 1111 pixels
Pixel size: 10 µm

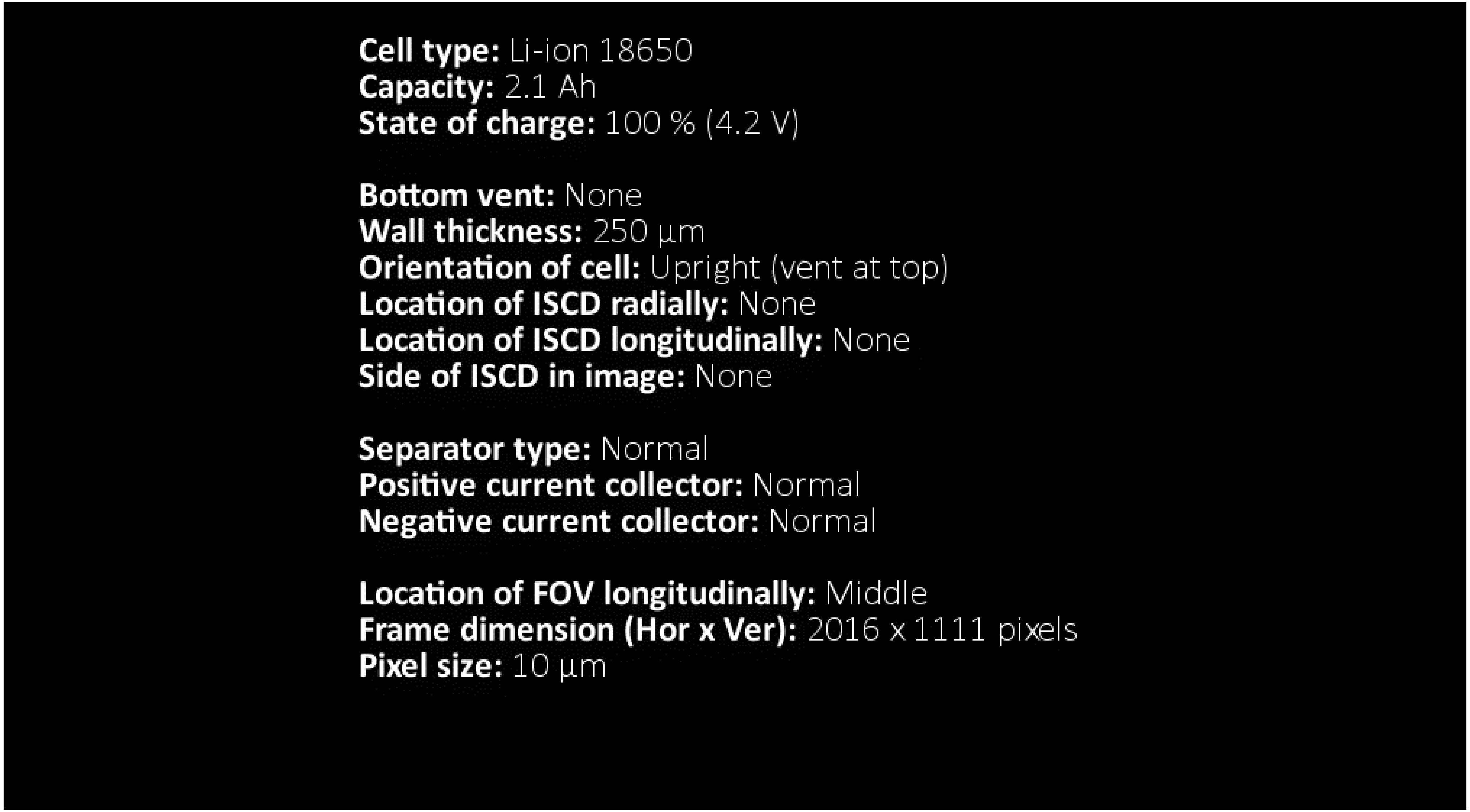
HIGH SPEED XRAY VIDEOGRAPHY



Cell type: Li-ion 18650
Capacity: 3.5 Ah
State of Charge: 100 % (4.2 V)
Bottom vent: No
Wall thickness: Not known
Separator: Polymer
Orientation of cell: Positive end up
Location of ISCD radially: N/A
Location of ISCD longitudinally: N/A
Side of ISCD in image: N/A

Location of FOV longitudinally: Top
Frame rate: 2000 Hz
Frame dimension (Hor x Ver): 1280 x 800 pixels
Pixel size: 17.8 µm

HIGH SPEED XRAY VIDEOGRAPHY



Cell type: Li-ion 18650
Capacity: 2.1 Ah
State of charge: 100 % (4.2 V)

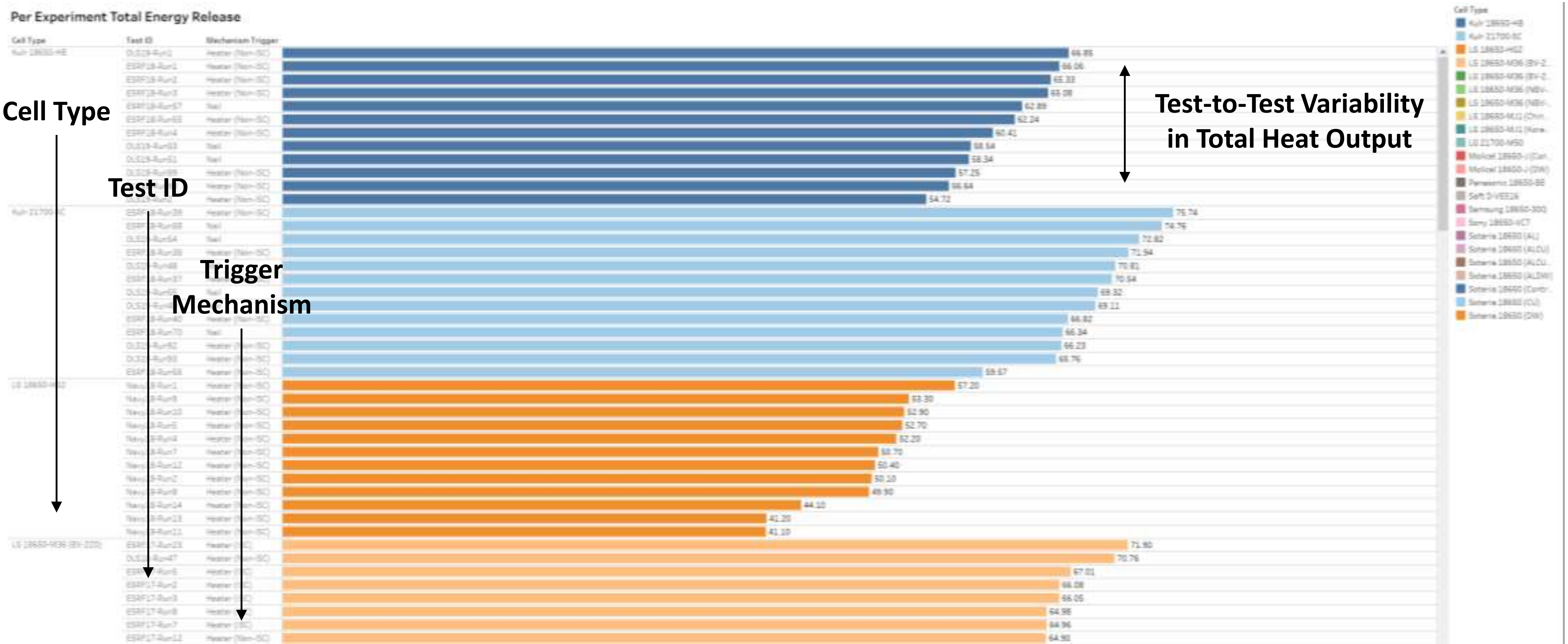
Bottom vent: None
Wall thickness: 250 µm
Orientation of cell: Upright (vent at top)
Location of ISCD radially: None
Location of ISCD longitudinally: None
Side of ISCD in image: None

Separator type: Normal
Positive current collector: Normal
Negative current collector: Normal

Location of FOV longitudinally: Middle
Frame dimension (Hor x Ver): 2016 x 1111 pixels
Pixel size: 10 µm

FTRC RESULTS: CHARACTERIZATION OF TOTAL ENERGY RELEASE

- Using Visual Analytics platform, Tableau, to compare data with rapid filtering capability; i.e. instantly compare based on cell type, trigger mechanism, failure mechanism, cell design variables, et…
- Since no two thermal runaway events are the same, test-to-test variability must be taken into consideration for any scientific effort that seeks to characterize the overall range of expected thermal runaway behavior for a given cell type



Cell Type

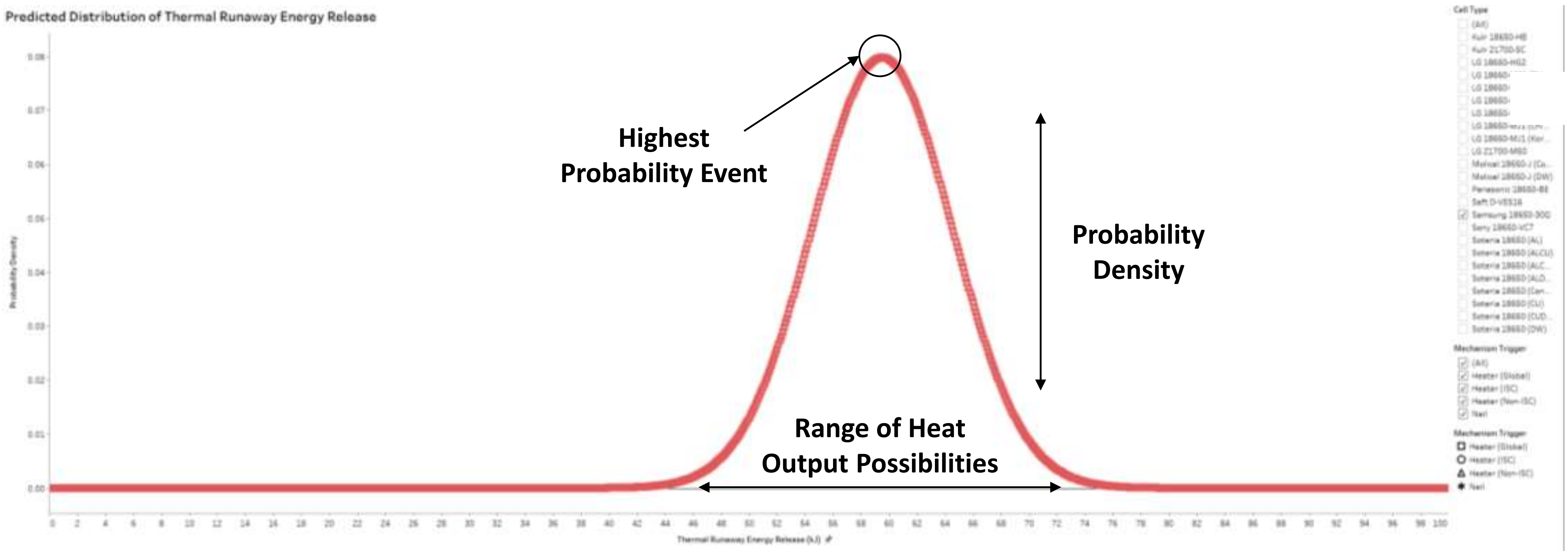
Test ID

Trigger Mechanism

Test-to-Test Variability in Total Heat Output

FTRC RESULTS: CHARACTERIZATION OF TOTAL ENERGY RELEASE

- **It is helpful to consider the variability of thermal runaway energy release as a statistical distribution to help answer the following questions:**
  - What is the highest probability energy release? What is the lowest?
  - What is the absolute maximum energy release one could expect? Minimum?
  - How do different cells, of similar capacities, compare in thermal runaway heat output?



Highest Probability Event

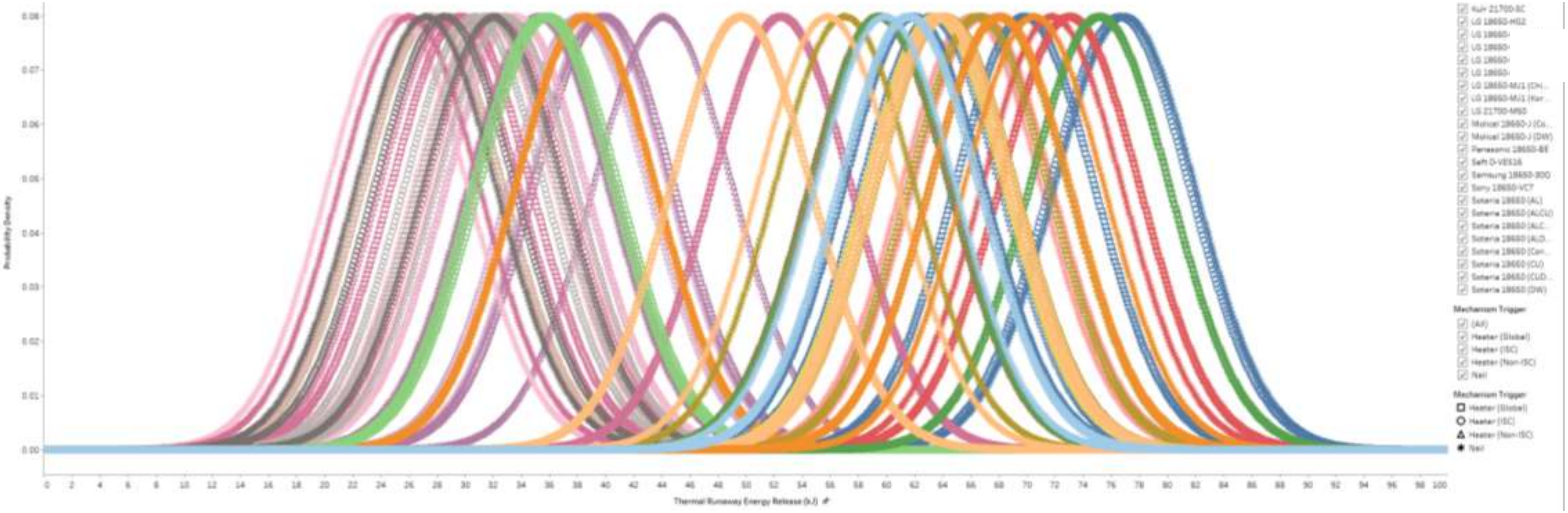
Probability Density

Range of Heat Output Possibilities

FTRC RESULTS: CHARACTERIZATION OF TOTAL ENERGY RELEASE

- **It is helpful to consider the variability of thermal runaway energy release as a statistical distribution to help answer the following questions:**
  - What is the highest probability energy release? What is the lowest?
  - What is the absolute maximum energy release one could expect? Minimum?
  - How do different cells, of similar capacities, compare in thermal runaway heat output?

Distributions for 24 cell types, spanning 3 cell formats, derived from 237 FTRC experiments



FTRC RESULTS: CHARACTERIZATION OF TOTAL ENERGY RELEASE

- In addition to consideration of test-to-test variability, average total heat output should be considered as a function of trigger mechanism; for this study we have heater trigger, internal short circuiting device (ISC) triggered, and nail penetration
- Nail penetration usually leads to the least violent thermal runaway events while heater induced thermal runaway results in more violent failures
- In some cases (Saft D-VES16), the internal short circuiting device results in the worst case failure

Cell Type

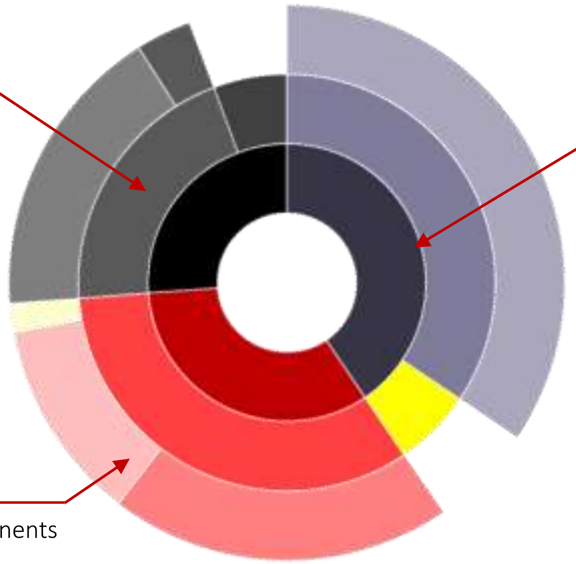
Trigger Mechanism

Heater Averages

Nail Average

FTRC RESULTS: ENERGY RELEASE FRACTIONS

- **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)



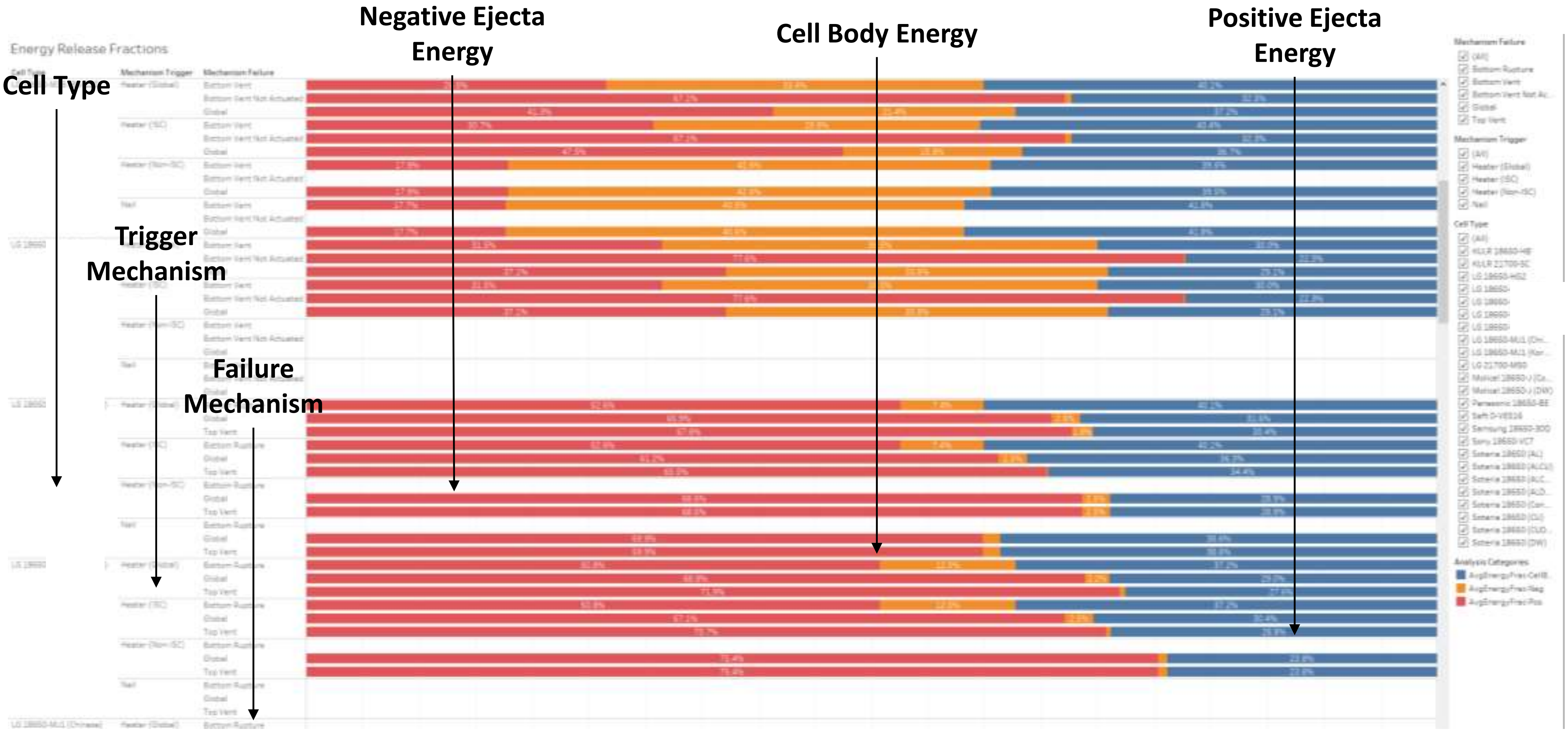
Middle Ring: Indicates calorimeter sub-assemblies

Inner Ring: Characterizes the division of total TR energy release where red corresponds to the cell casing, indigo to the positive ejecta and gases, and black to the negative ejecta and gases

Outer Ring: Corresponds to components of the calorimeter sub-assemblies

FTRC RESULTS: ENERGY RELEASE FRACTIONS

- Very important to consider the energy release fractions as a function of BOTH trigger mechanism and failure mechanism



Cell Type

Trigger Mechanism

Failure Mechanism

Negative Ejecta Energy

Cell Body Energy

Positive Ejecta Energy

SUMMARY

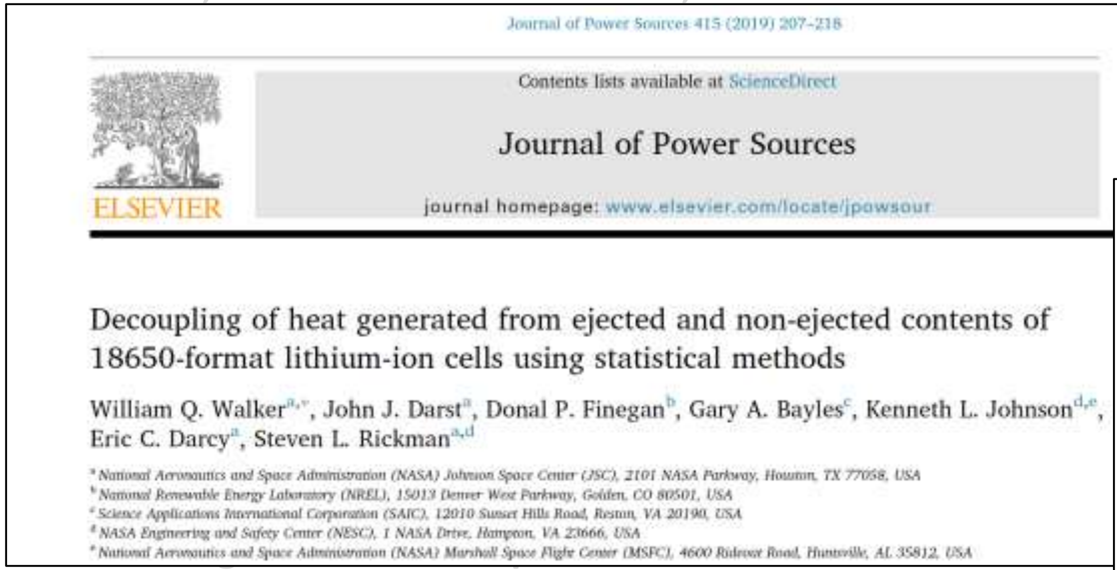
- **FTRC techniques and the associated results provide the means to develop optimized Li-ion batteries while also maintaining necessary safety and margin**
- **FTRC, and the associated results, enables the discernment of the fractions of thermal runaway energy released through the cell casing and through 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
- **There is not a linear correlation between stored electrochemical energy and total thermal runaway heat output**
- **Thermal runaway behavior should always be considered as a function of:**
  - Cell format and associated design variables
  - Trigger mechanism and failure mechanism (i.e. top vent, bottom vent, side wall rupture, spin groove breach, et…)
  - Test-to-test variability and the associated statistical distribution
  - Both as TOTAL energy release and as energy release FRACTIONS
- **Recent findings suggest that thermal runaway heat output should be considered as a function of cell lot**
- **Average total heat output should be considered as a function of trigger mechanism:**
  - Nail penetration usually leads to the least violent thermal runaway events while heater induced thermal runaway results in more violent failures
  - In some cases (Saft D-VES16), the internal short circuiting device results in the worst case failure

SUMMARY

- FTRC techniques and the associated results provide the means to develop optimized Li-ion batteries while also maintaining necessary safety and margin
- FTRC, and the associated results, enables the discernment of the fractions of thermal runaway energy released through the cell

10 runs to establish statistically defendable results

hen they remain intact



Journal of Power Sources 415 (2019) 207–218

Contents lists available at ScienceDirect

Journal of Power Sources

journal homepage: www.elsevier.com/locate/jpowsour

Decoupling of heat generated from ejected and non-ejected contents of 18650-format lithium-ion cells using statistical methods

William Q. Walker[a,*], John J. Darst[a], Donal P. Finegan[b], Gary A. Bayles[c], Kenneth L. Johnson[d,e], Eric C. Darcy[a], Steven L. Rickman[a,d]

[a] National Aeronautics and Space Administration (NASA) Johnson Space Center (JSC), 2101 NASA Parkway, Houston, TX 77058, USA
[b] National Renewable Energy Laboratory (NREL), 15013 Denver West Parkway, Golden, CO 80501, USA
[c] Science Applications International Corporation (SAIC), 12010 Sunset Hills Road, Reston, VA 20190, USA
[d] NASA Engineering and Safety Center (NESC), 1 NASA Drive, Hampton, VA 23666, USA
[e] National Aeronautics and Space Administration (NASA) Marshall Space Flight Center (MSFC), 4600 Rideout Road, Huntsville, AL 35812, USA

Journal of Power Sources 417 (2019) 29–41

Contents lists available at ScienceDirect

Journal of Power Sources

journal homepage: www.elsevier.com/locate/jpowsour

Modelling and experiments to identify high-risk failure scenarios for testing the safety of lithium-ion cells

Donal P. Finegan[a,*], John Darst[b], William Walker[b], Qibo Li[a], Chuanbo Yang[a], Rhodri Jervis[c], Thomas M.M. Heenan[c], Jennifer Hack[c], James C. Thomas[b], Alexander Rack[d], Dan J.L. Brett[c], Paul R. Shearing[c], Matt Keyser[a], Eric Darcy[b]

[a] National Renewable Energy Laboratory, 15013 Denver W Parkway, Golden, CO, 80401, USA
[b] NASA Johnson Space Center, 2101 E NASA Pkwy, Houston, TX, 77058, USA
[c] Electrochemical Innovation Lab, Department of Chemical Engineering, University College London, London, WC1E 7JE, UK
[d] The European Synchrotron (ESRF), 71 Avenue des Martyrs, 38000, Grenoble, France

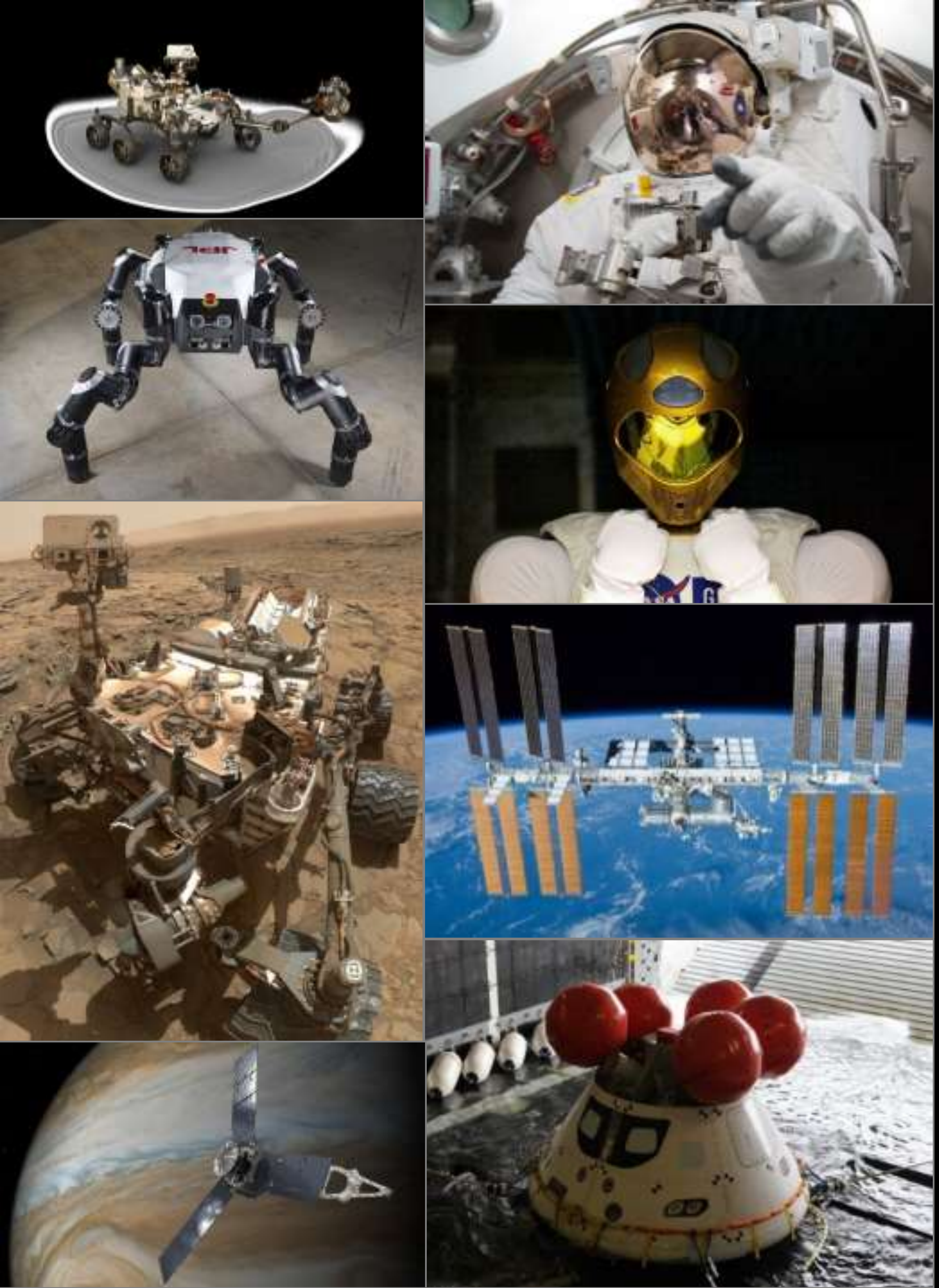
  - Nail penetration usually leads to the least violent thermal ru
  - In some cases (Saft D-VES16), the internal short circuiting d

SNEAK PREVIEW OF NEW CAPABILITIES

- **Actively working to address the unique challenges associated with pouch cell thermal runaway events which requires a substantially different FTRC architecture**
- **Not all applications utilize small format Li-ion cells – another effort is underway to develop FTRC for cell's with capacities >100 Ah**

ACKNOWLEDGEMENTS

- **NASA Engineering and Safety Center**
  - Steve Rickman and Christopher Iannello, Ph.D.
- **NASA JSC Engineering Directorate (EA):**
  - Power and Propulsion Division (EP)
  - Structural Engineering Division (ES)
- **National Renewable Energy Laboratory (NREL)**
- **FTRC Team Members**
- **NASA JSC Energy Systems Test Area (ESTA)**
- **Diamond Light Source (DLS) Facility**
- **European Synchrotron Radiation Facility (ESRF)**



QUESTIONS?