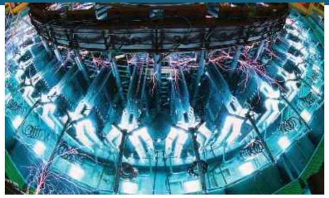
SAND2020-1909PE

2540 POWER SOURCES TECHNOLOGY GROUP

CENTER 2500

CSEP

COMPONENT SCIENCE, ENGINEERING, & PRODUCTION



Power Sources Technology Group Overview

February 17, 2020

PRESENTED BY

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Principle Member of Technical Staff

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Power Sources Technology Group

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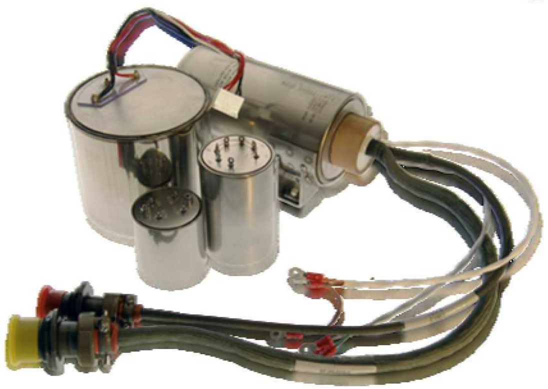
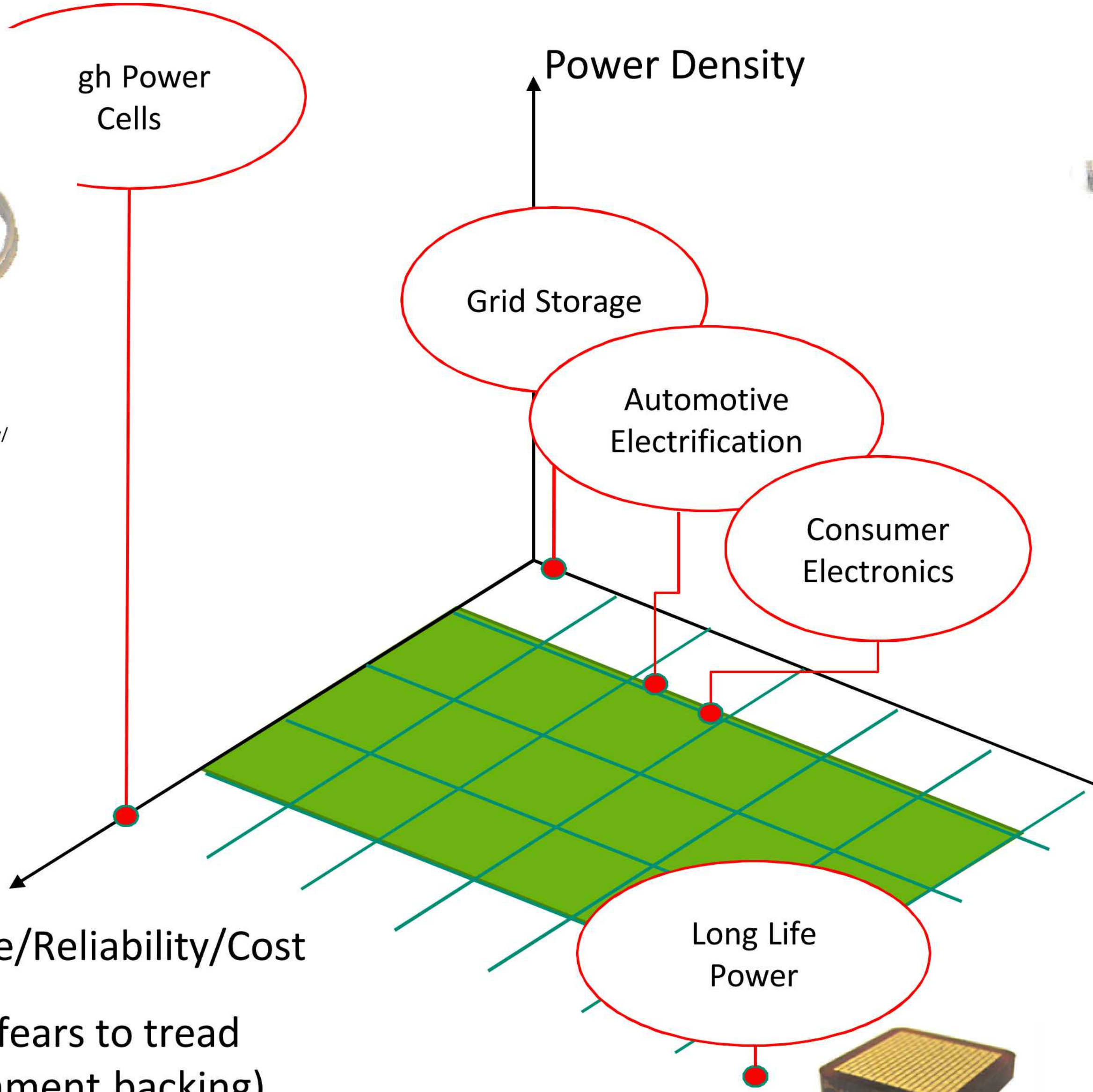


https://www.eaglepicher.com/technology/battery-chemistries/thermal-battery/

Thermal Battery
- 3 cc
- 30V, 10A, 2 sec

~300 W or
~50 Whr/L

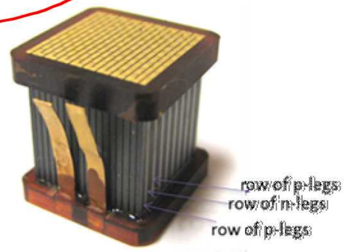


Smartphone Battery
- 15 cc
- 3V, 1A, 5 hr

~3 W or
~1000 Whr/L

Where industry fears to tread
(without government backing)

Thermoelectric
- 500 cc
- 3V, 5 mA, 40 years



~0.015 W or
~10,000 Whr/L

*Slide content courtesy of Chris Apblett (caapble@sandia.gov)

Power Sources Technology Group (PSTG) at Sandia, NM

Develops, delivers, and assures the performance of power source components for nuclear weapons and innovative solutions for other national security challenges. The PSTG utilizes the latest scientific and engineering technologies to research, design, develop, and produce power sources used for NNSA, DoD, DOE, NASA, and commercial applications.

- Divided into five departments by topic area
  - Research and Development (surveillance, new chemistries, vehicle and power systems, abuse testing)
  - Design and Development (lithium primary and secondary)
  - Design and Development (thermal)
  - Production (lithium primary and secondary, reserve, thermal)
  - Special Projects (thermoelectrics)
- Multi-disciplinary approach
  - Mechanical Engineering
  - Chemical Engineering
  - Electrical Engineering
  - Chemistry
  - Materials Science

System Drivers and Performance Attributes

Cost | Schedule | Weight | Volume | Power | Energy | Safety | Environments

Critical Technology Areas

Products
- Reserve Batteries • Primary Batteries
- Secondary Batteries • Energy Conversion
- Ultracapacitors • Battery Safety • Diagnostics

Technologies
- Thermal Batteries • Lithium Primary Batteries • Thermoelectrics • Power Sources • Lithium-Ion Batteries
- Conversion Technologies

Materials
- MgO • FeS_2 • MnO_2 • CoS_2 • Li-Si • Li • C
- Si • LiB • Insulation • Electrolyte Salts/Solvents • Package Hardware

Processes
- Seals and Welding • Pellet Pressing • Coating • Mixing
- Material Shaping and Printing
- CAD Design/Modelling

Manufacturability
- Electrochemical Materials
- Packaging Materials
- Thermal Management Materials

Supply Chain
- Procurement • Tier 1 Suppliers
- Tier 2 Suppliers • Materials / Piece Parts

Modeling and Simulation
- Thermal (inc. TABS)
- Electrochemical • Mechanical
- First Principles

Capabilities

Facilities and Tools

FABRICATION
- Electrode Coating • Pelletization • Battery Prototyping • 3D Printing • BMS Electronics • Chemical Synthesis • Dry Room • CAD Modeling

CHARACTERIZATION
- BATLab • Electrochemical Characterization
- Calorimetry • Gas Analysis • Spectroscopy and Microscopy • Thermal/Mechanical environments • Modeling

Competencies and Expertise
- Battery Design and Engineering
- Battery Manufacturing
- Battery Safety and Abuse Testing
- Electrode Coating
- Thermal Management
- Modeling/Simulation
- Material Synthesis
- Material Science
- Energy Harvesting
- Battery Management System Design

Technologies Areas
- Transportation Energy Storage Performance and Safety
- Grid Energy Storage Performance and Safety
- Thermoelectrics
- Battery Safety Science
- Thermal Battery R&D
- Surveillance (Aging Phenomena and Life Predictions)
- Modeling (Mechanics, Thermal, Thermodynamics, and Safety)

Technology Drivers

Customer Needs
- Liquid Reserve Batteries
- Conventional Munition Reserve Power Sources (DOD)
- Autonomous Power
- Long Life Power
- Advanced Energy Dense Materials
- *In-situ* degradation monitoring
- Understanding Aging Phenomena

Capability/Competency Gap
- Aging Facilities Infrastructure
- Environmental Test Resources (Vibration, Shock, Thermal)
- Component Development Infrastructure

Technology Area Gap
- Shortened Development Cycles
- More Energy Density and SWaP
- More Flexible and Agile Design
- Predictive Capabilities (Aging, Life, Safety)
- Improved Diagnostics (*in-situ* and *ex-situ*)

PSTG Portfolio

ND

Weapon Engineering & Production (WE&P)

Advanced & Exploratory

Power Source Design

Power Source Production

Surveillance

Security

DoD Joint Munitions Program

Strategic Partnership Programs

Mobility

Vehicle Technologies Office

Joint Center for Energy Storage Research

Strategic Partnership Programs

Stationary Storage

Office of Electricity

LDRD

Strategic Partnership Programs

Energy Storage Technologies

Core Competencies and Capabilities

Program Support & Collaborations

Categories of Power Sources Technology

Electrochemical

Li-Ambient Power Sources (MnO_2, SO_2, $SOCl_2$,FeS_2)

- High current and voltage
- Instant on (~)
- Limited shelf life
- Limited active life

Reserve Power Sources (AgO/Zn, $Li/SOCl_2/SO_2Cl_2$)

- High current and voltage
- Delay time for power
- Moderate shelf life
- Limited active life

Thermal Batteries (Li/FeS_2, $LiCoS_2$, $Ca/CaCrO_4$)

- Moderate current and voltage
- Delay time for power
- Long shelf life
- Limited active life

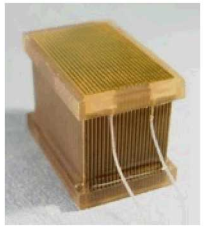
Lithium-Ion Power Sources (Graphite/Metal Oxide)

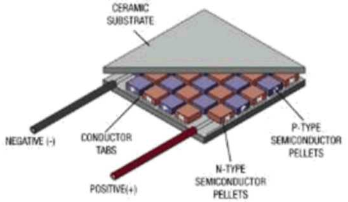
- High current and voltage
- 1000s of recharge cycles
- Limited shelf life
- Safety concerns due to flammable electrolyte
- High depth of discharge
- No memory effects seen in other secondary chemistries

Thermoelectric

Thermal Electric Power Sources (SiGe, BiTe + fuel)

- Low current and voltage
- Instant on
- Long shelf life
- Long active life





Simple Schematic of a Thermal Battery Cell

Pellets (or pills) are pressed from powder

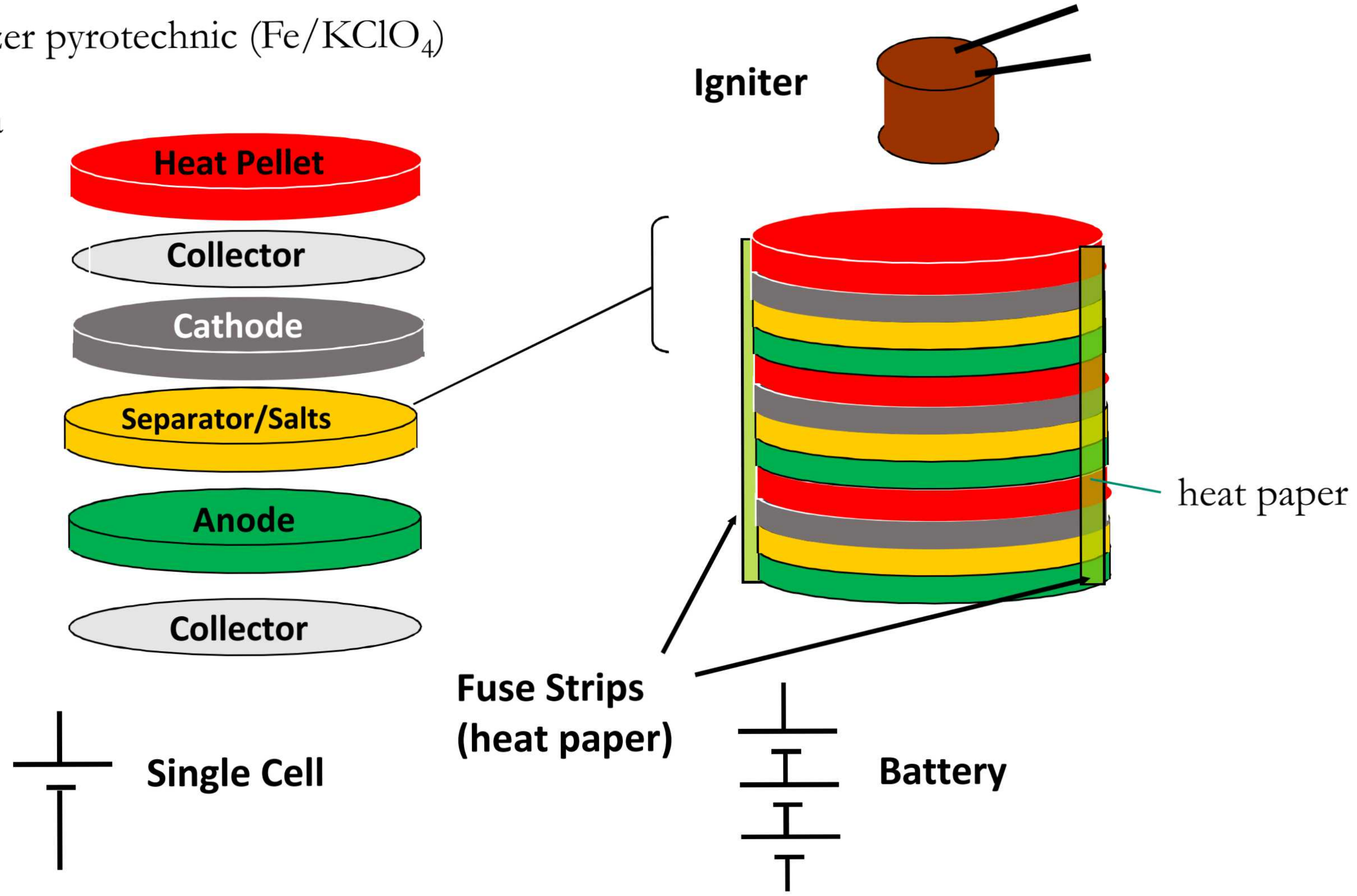
Heat generation = metal/oxidizer pyrotechnic ($Fe/KClO_4$)

Collector = metal layer acts as a heat buffer

Cathode = FeS_2 or CoS_2 provides reductant

Separator = salts and a physical carrier provides “solvent” and ionic conduction pathway

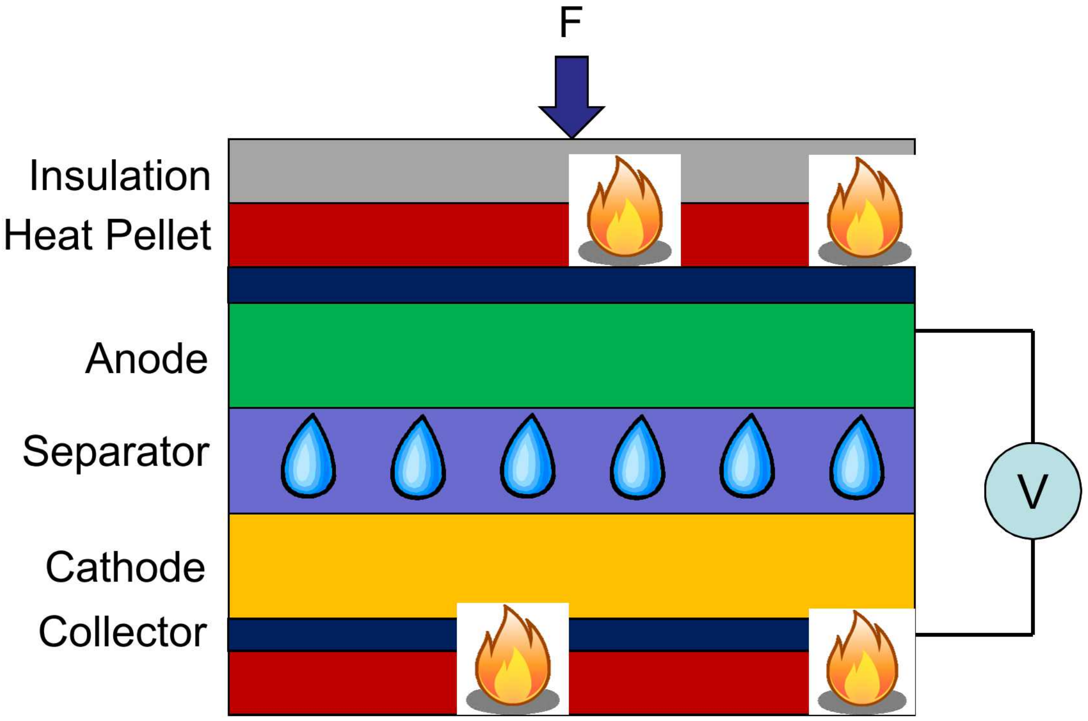
Anode = Li-Si eutectic mix provides oxidant

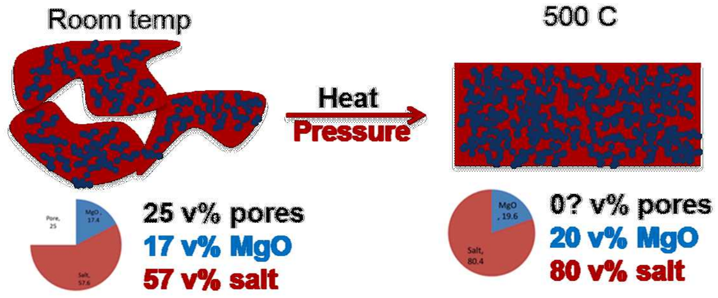


Center-fire, no heat paper; central hole, faster rise time.

Physical mechanisms in thermal batteries

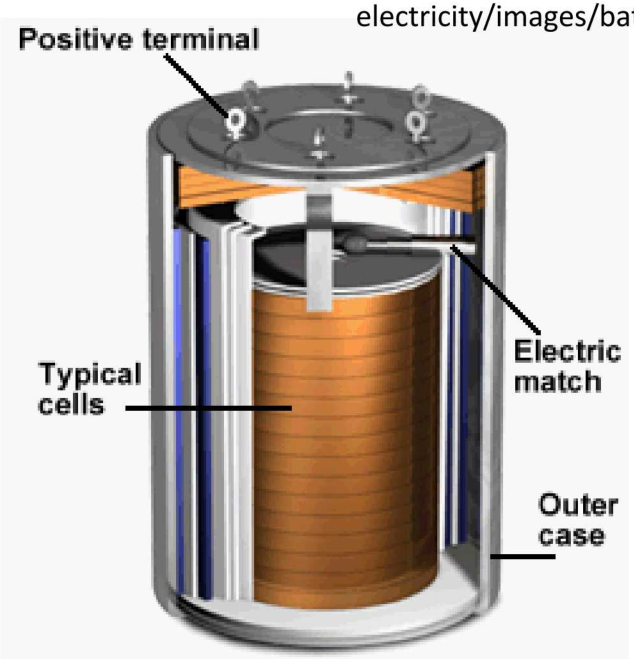
- Battery activation is a complicated, multi-step process
  - Heat pellet burning
  - Thermal diffusion
  - Melting of the electrolyte
  - Deformation of the separator
  - Rebound of the insulation
  - Flow of the electrolyte
  - Activation
- Why performance models of thermal batteries?
  - Predict activation times
  - Predict electrochemical performance
  - Optimize volume, insulation, manufacturing
  - Understand system-level effects





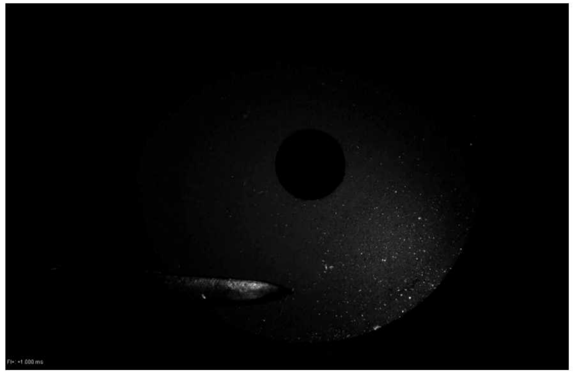
- Thermal battery activation is a true multi-physics process!

Thermal Batteries



https://micro.magnet.fsu.edu/electromag/electricity/images/batteries/thermal.gif

- High temperature operation
- Large temperature range
- 10s to 100s of volts
- High current
- Negligible self discharge
- Solid state only
- Hermetically sealed
- 20+ yr shelf life
- Requires activation (delay)
- Single use
- Isolated (usually) from can
- Expensive due to volume



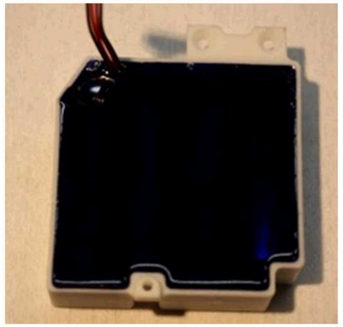
$Fe-KClO_4$ pellet

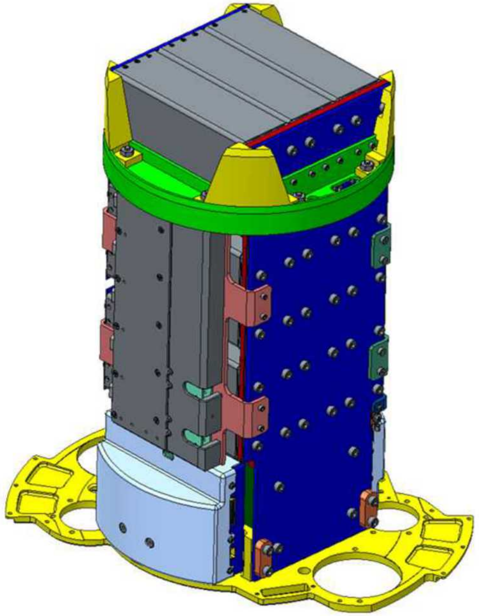
Ni-Al pellet

*Videos courtesy of Chris Apblett (caapble@sandia.gov) and David Ingersoll (dingers@sandia.gov)

Ambient Temperature Li-Primary or Li-ion Batteries

- Commercially available Li-CF_x, Li-$SOCl_2$, or Li-MnO_2 cells connected in series/parallel configuration with or without encapsulation
- Use of COTS parts has advantages (high capacity/power, wide temperature range, parallel strings for redundancy)
- Challenges due to low visibility into manufacturing
- Can be designed to provide main power for flight tests, telemetry, code management, and other non-initiation train power
- Batteries need to be certified for lifetime and performance in shock, vibe, and thermal environments
- Design challenges include weld reproducibility, encapsulant use, volume/form factor
- Wide variety of power source solutions are achievable
  - <10V to >100 V
  - mA to >100A
  - <1 Ahr to >10Ahr



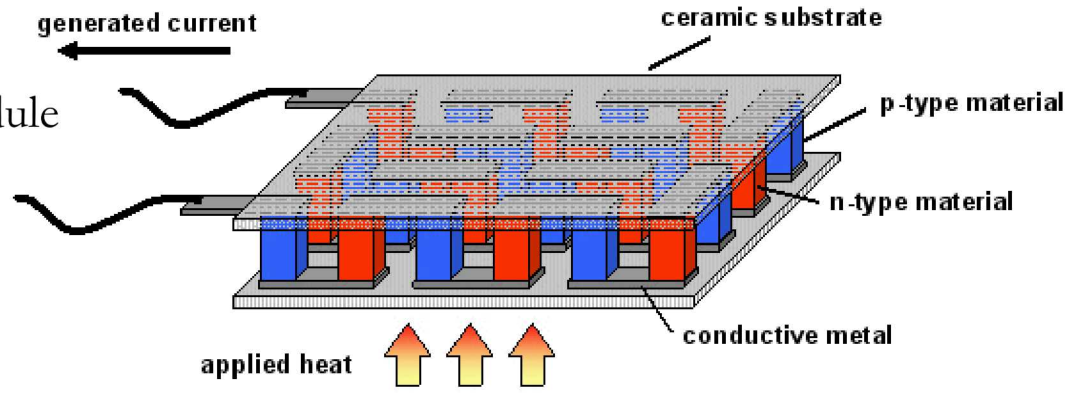


Long-Life Power Sources

- Conversion of heat to electricity via the Seebeck effect
  - Heat from α decay of ^{238}Pu flows through thermoelectric module
  - Waste heat “scavenged” from other sources
- Advantages
  - No moving parts
  - Passive power generation
  - Long-life
  - High reliability
  - Insensitive to temperature extremes
  - Small volume

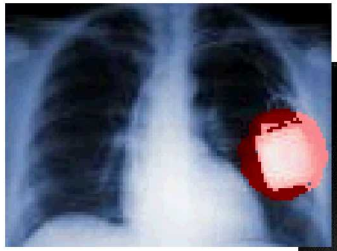
$$ZT = S^2\sigma T/\kappa$$

S = Seebeck coefficient
σ = electrical conductivity
κ = thermal conductivity
T = absolute temperature

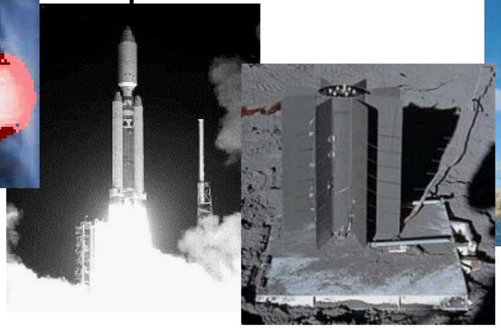


https://www.sigmaaldrich.com/content/dam/sigma-aldrich/materials-science/metal-ceramic-science/thermoelectric-module.jpg

Pacemakers



Space Power



Lighthouses

Thermoelectric Materials

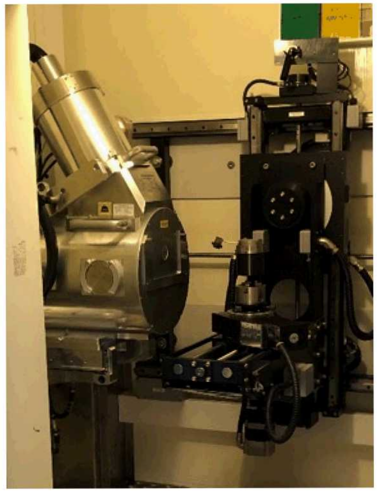
SiGe (alloy)
~1000º C, ZT of ~0.7

Bi_2Te_3
~ 250º C, ZT of ~0.9-1.1

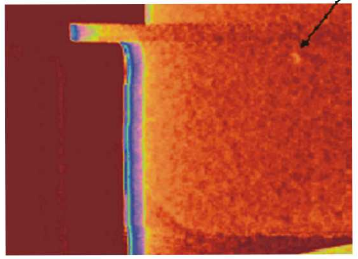
NASA RHU Pellet

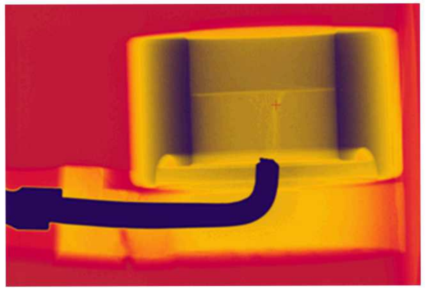
Inspection and Electrical Testing

- Visual weld/GTM seal inspection (leak paths)
- Discharge Testing
  - Single cell
  - Full battery
- Non-D electrical (V standoff)
- X-ray/CT
  - Build errors
  - Anomaly investigations



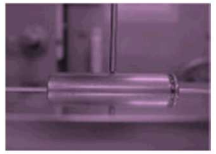
Inclusion, $\Delta\rho = 0.152\ g/cm^3$

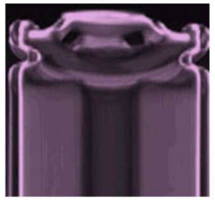




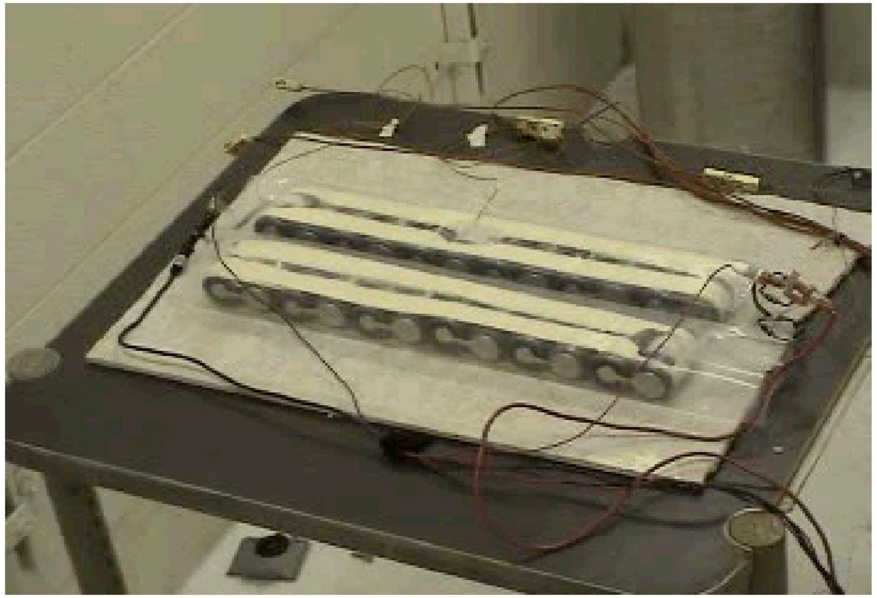
SNL Battery Abuse Testing Laboratory (BATLab)

- Comprehensive abuse testing of cells, batteries and systems from mWh to kWh
- Mechanical abuse
  - Penetration
  - Crush
  - Impact
  - Immersion
- Thermal abuse
  - Over temperature
  - Flammability measurements
  - Thermal propagation
  - Calorimetry
- Electrical abuse
  - Overvoltage/overcharge
  - Short circuit
  - Overdischarge/voltage reversal





Overcharge Test



Charging with Reversed Polarity

Battery Abuse Testing – System Field Failures

Tesla Model S fire in October 2013, where the fire was isolated to the front portion of the vehicle and did not propagate through the entire battery

Any **single point failure** that **propagates** through an entire battery system is an **unacceptable** scenario to ensure battery safety

Field failures could include:

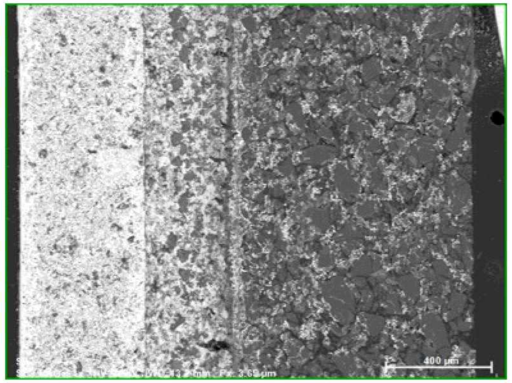
- Latent manufacturing defects
- Internal short circuits
- Unique use or **abuse conditions**
- Control failure (low voltage, control systems, connectors, boards, not battery initiated)

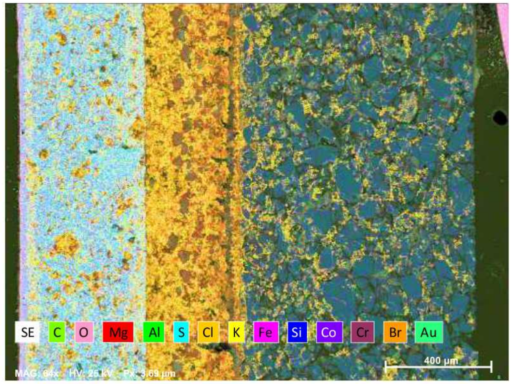
Thermal Abuse Test

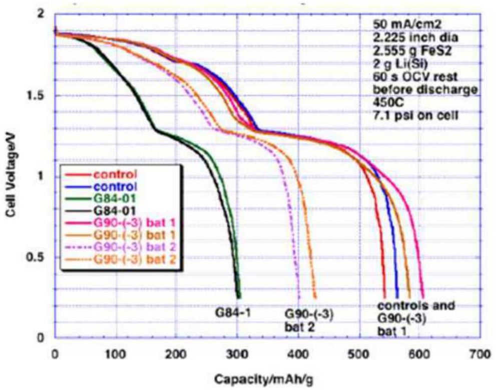
Failure Propagation (0-40s, 1min)

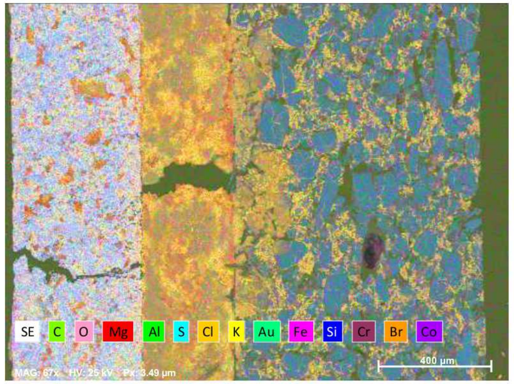
Research and Development Tools

- Chemical analysis (what and how much is present?)
  - ICP
  - Differential Scanning Calorimetry
  - Thermogravimetric Analysis
- Pyrotechnic analysis (how much energy? how sensitive? how fast?)
  - Bomb Calorimetry
  - Ignition Sensitivity
  - Burn Speed
- Microanalysis with EDS (what's the distribution of elements?)
  - Type and nature of mechanisms of electrochemical reactions
  - Aging trends vs manufacturing variability
- Gas sampling (what are the reaction products? how much?)
  - Provides insight into aging characteristics
- X-Ray and CT inspection (what's inside? evidence of anomaly?)
  - Provides non-destructive inspection data for pristine and spent units







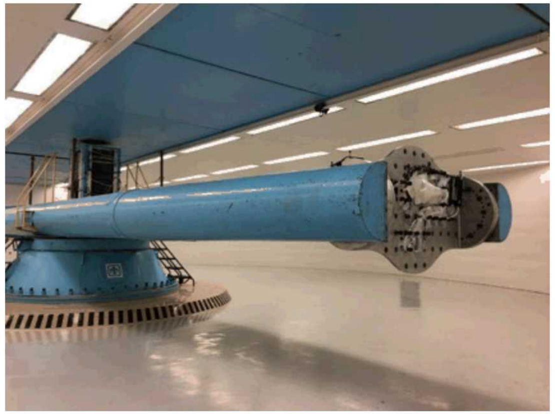


Battery level and single cell testing provide key data on battery performance and reliability.

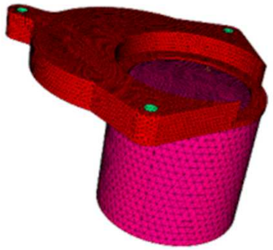
Gas sampling and analysis identify oxygen and water content that can degrade cathode and anode.

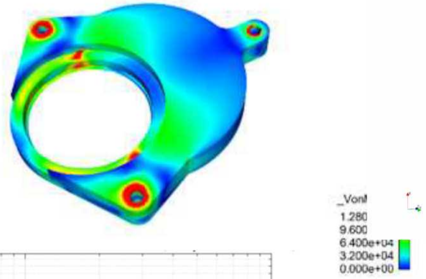
Research and Development Tools

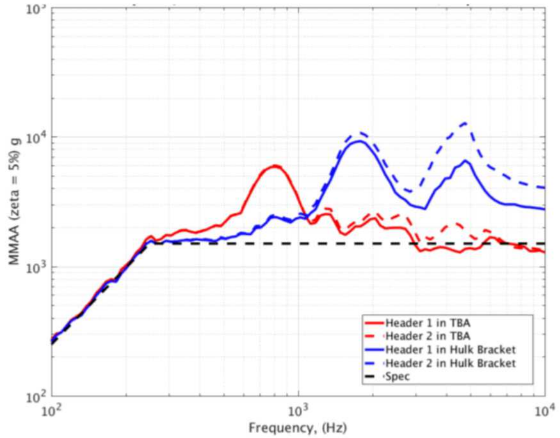
- Qualification to Environments
  - Shock
  - Vibration
  - Acceleration
  - Thermal
  - Combined environments
- Modeling and Simulation
  - Modal analysis
  - Finite element
  - Thermal modeling

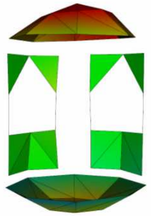


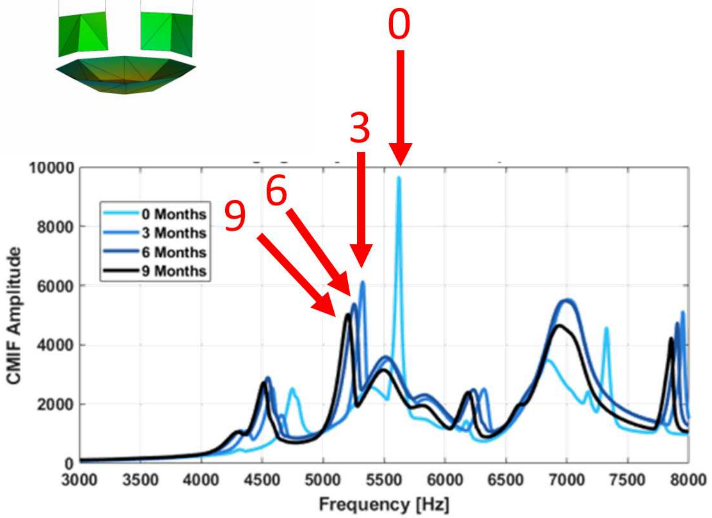
https://tours.sandia.gov/Superfuge/







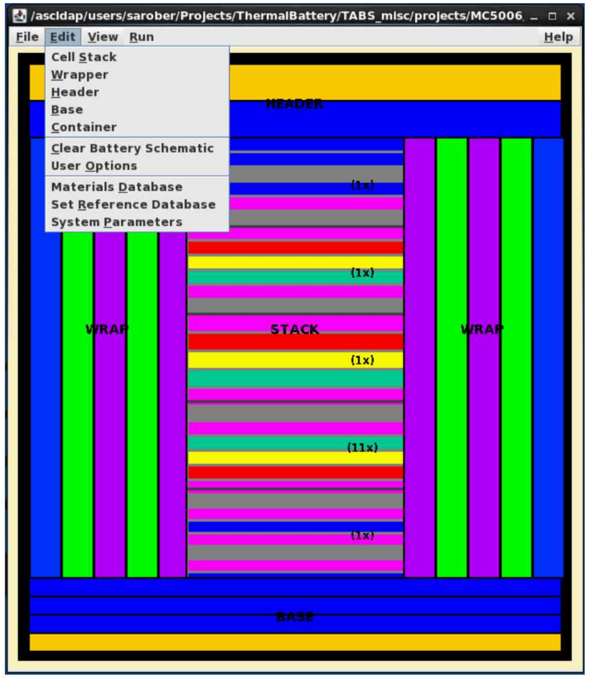




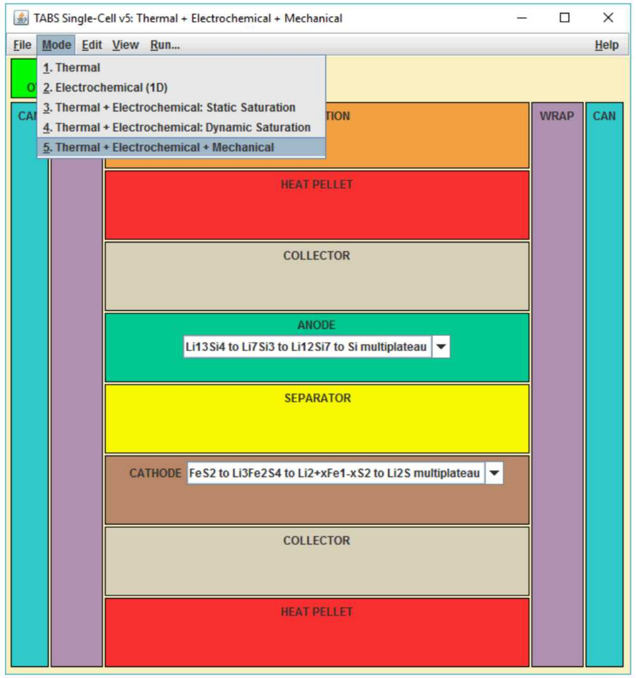
TABS: The Thermally Activated Battery Simulator

*TABS content courtesy of Ed Piekos (espieko@sandia.gov) and Scott Roberts (sarober@sandia.gov)

- TABS design principles
  - Create a user interface **intuitive to battery designers**, not just for computational scientists
  - Be **computationally efficient**, so many design iterations can be explored in a single work day
  - Present the user with the most **relevant quantities of interest**, yet enable them to explore more deeply
  - Have **demonstrated credibility**, such that the user knows when and how much to trust the solutions



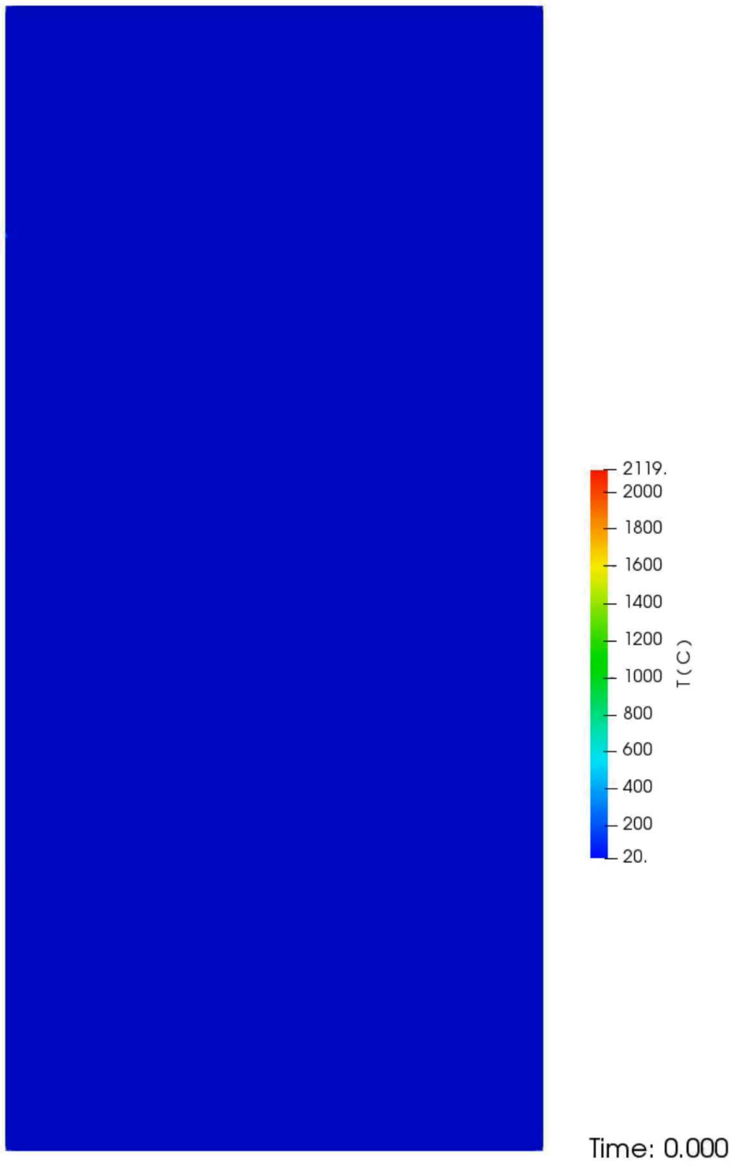
TABS-FB: Full Battery
- Thermal



TABS-SC: Single Cell
- Thermal
- Mechanical
- Flow
- Electrochemical

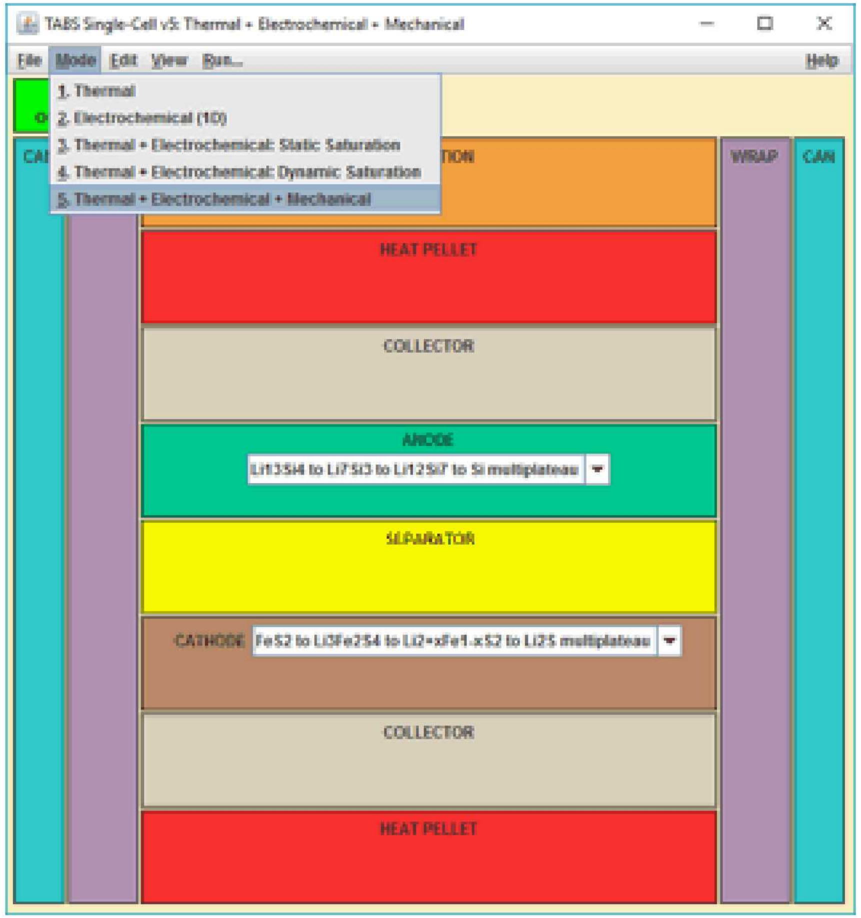
- Two powerful performance/design models with an easy-to-use interface

Running a TABS full battery thermal simulation



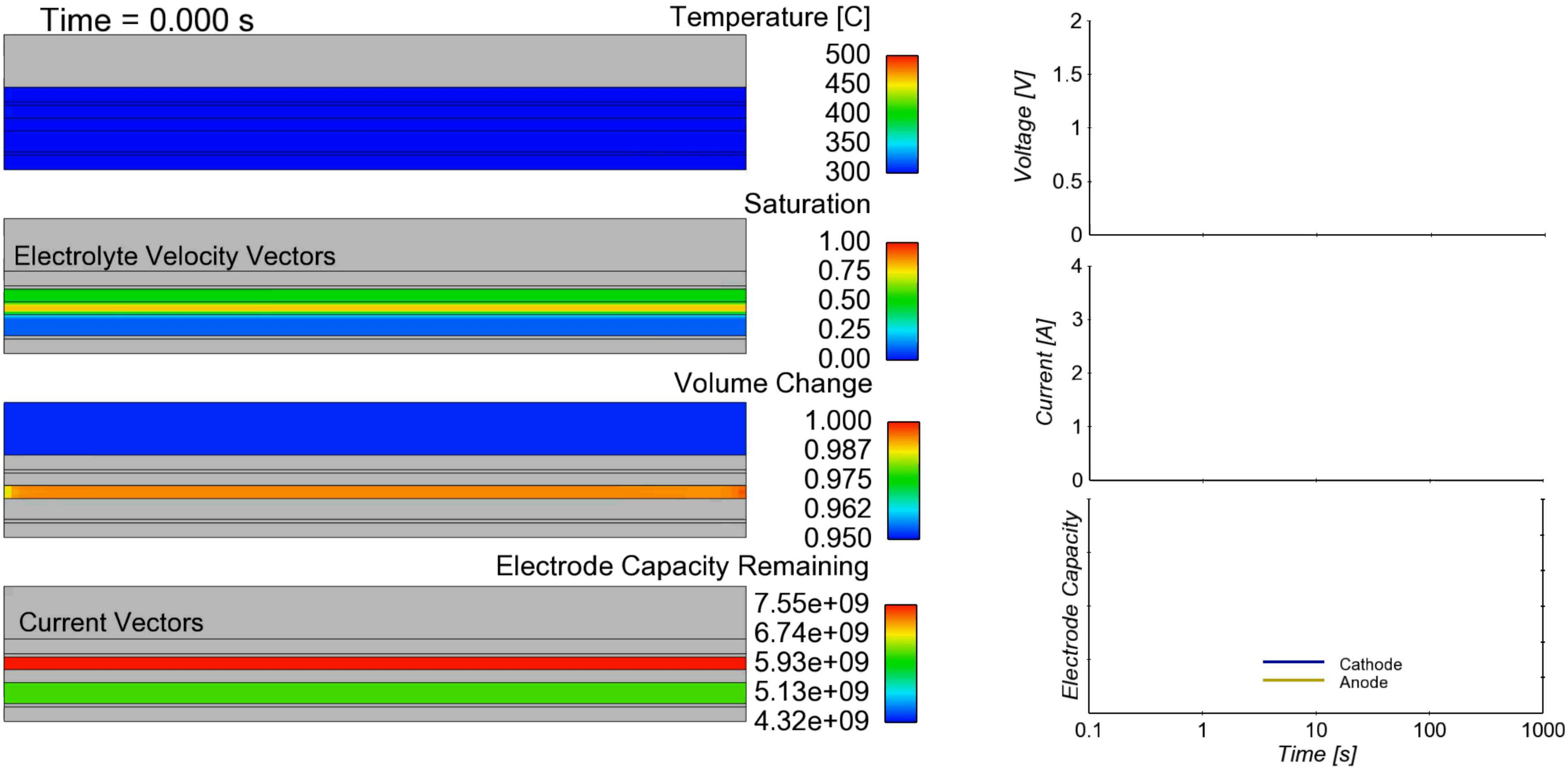
Setting up an electrochemical simulation in TABS-SC

- TABS-SC brings electrochemical (current/voltage) predictions
  - Thermal: Heat generation (burning, Joule) and transport
  - Fluid: Two-phase porous flow in anode/separator/cathode
  - Mechanical: Separator deformation, insulation rebound, stack force
  - Electrochemistry: Species diffusion, electrical transport, sub-grid multi-plateau electrochemical reactions
- Multiple fidelity modes (details in next talk, Voskuilen):
  - 1: Thermal
  - 2: Electrochemical (1D)
  - 3: Static partially saturated fluid + thermal + electrochemical
  - 4: Fluid + thermal + electrochemical
  - 5: Fluid + thermal + electrochemical + mechanical
- Same easy setup at TABS-FB!

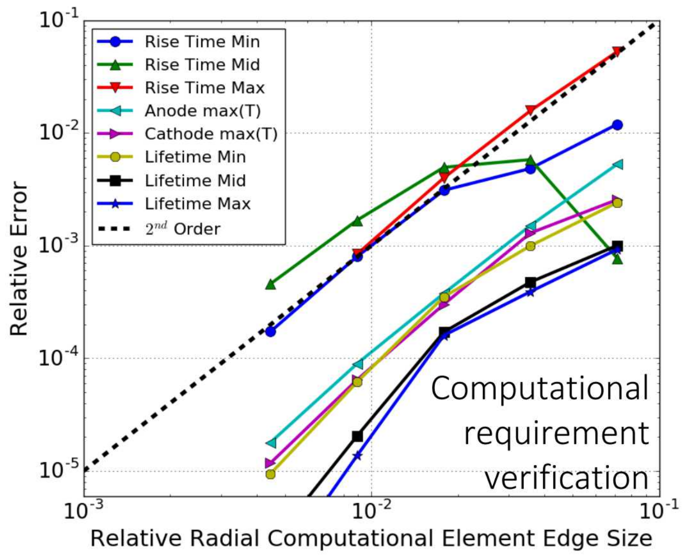


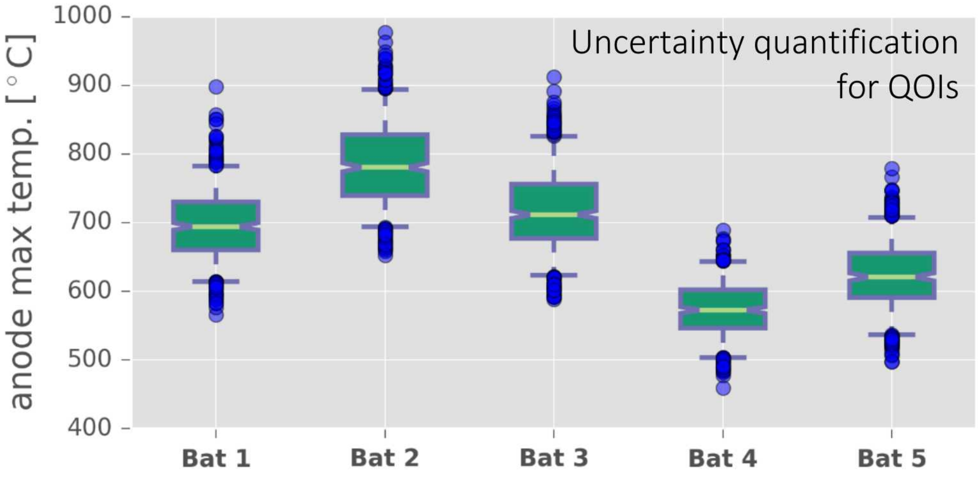
- TABS-SC is multi-physics solver for current and voltage at the single-cell scale

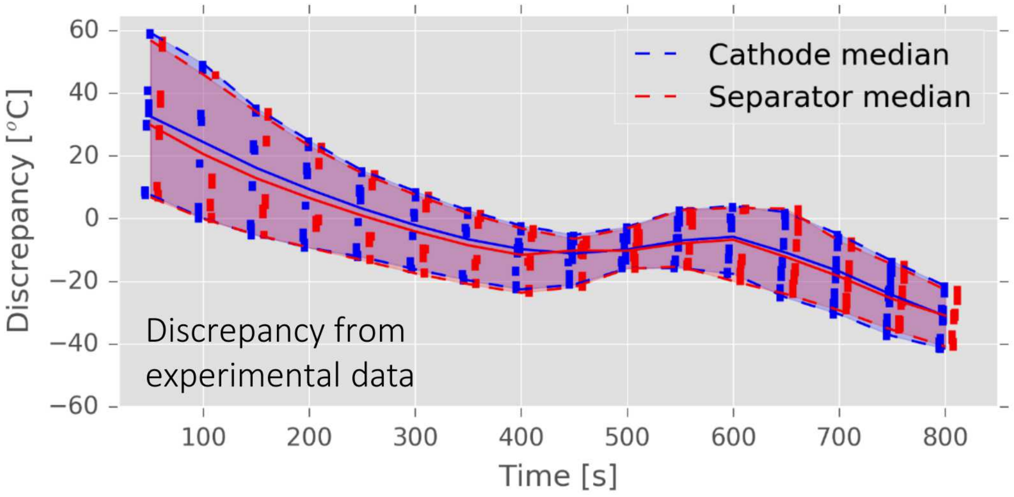
TABS-SC multi-physics visualization demonstration

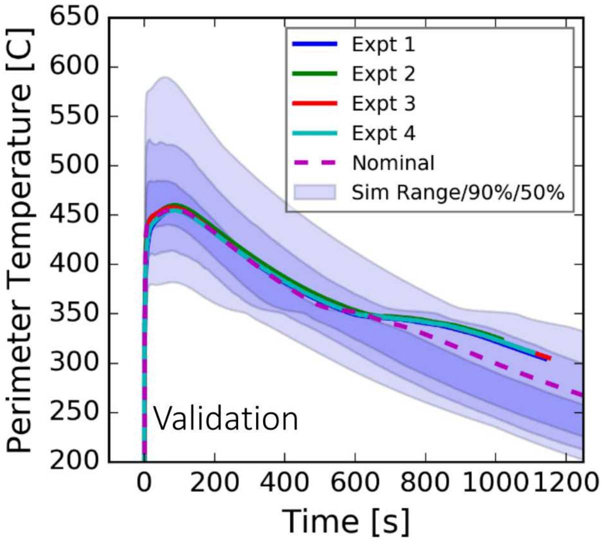


TABS-FB credibility assessment







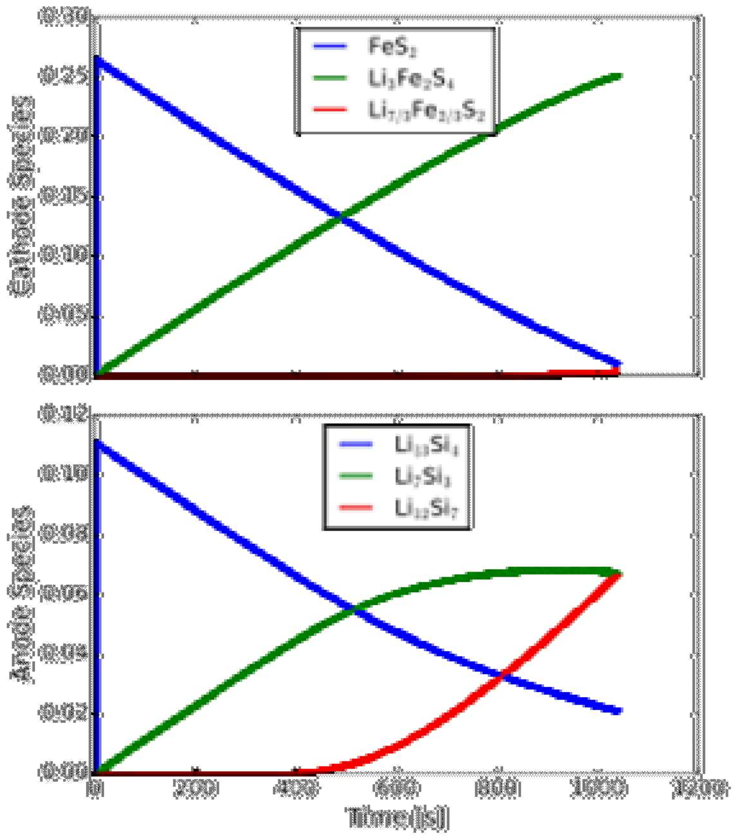


- Verification, validation, and uncertainty quantification (V&V/UQ) establish model credibility

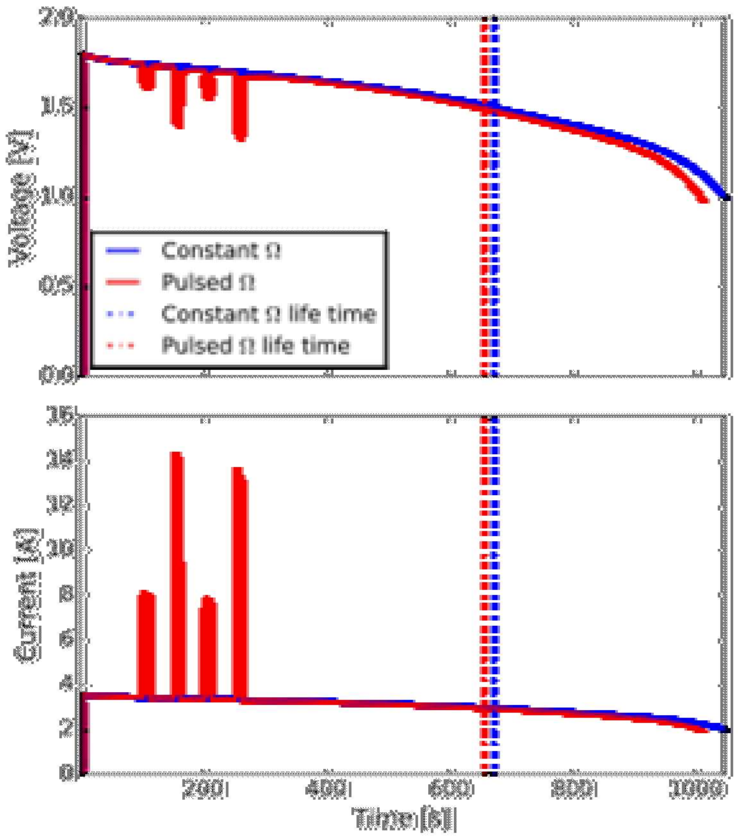
Additional quantities of interest from TABS-SC

QOI	Value
Rise time (@1.5V)	0.425 s
Lifetime (@1.5V)	691 s
Max Anode T	507 C
Max Cathode T	483 C
Max Voltage	1.80 V
Max Current	3.59 A
Separator Strain	16.3%

Scalar QOIs represent quick look at first-order design parameters. Predictions all in expected ranges



Reactions in cathode are fast, while anode access multiple simultaneous reaction plateaus



Pulses accelerate reactions and reduce life time

- Valuable design insight post-processed from simulation results, immediately available in Excel file

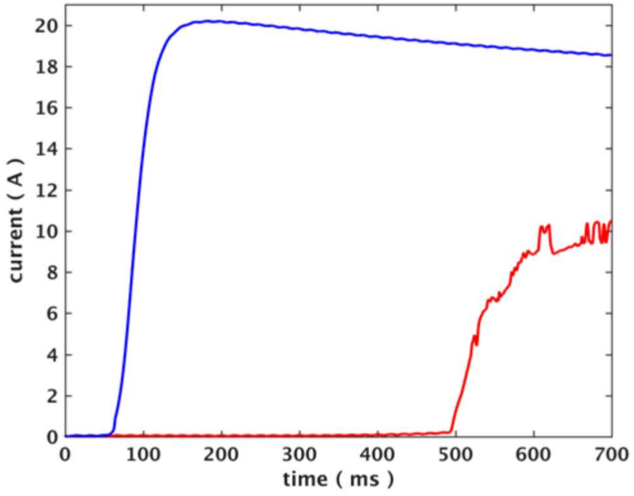
Summary

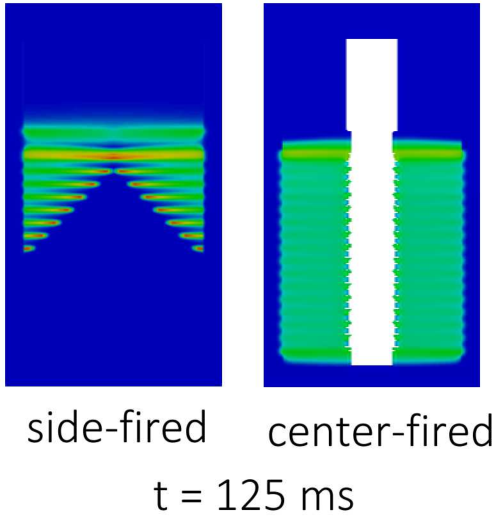
- Engineering and science in the power sources field is strongly multidisciplinary
  - Heat transfer
  - Electrochemistry
  - Material behavior
  - Fluid flow
  - Mass transport
  - Electrical circuits
  - Materials Science (polymers)
  - Materials Science (metallurgy)
  - Chemistry (aging)
  - Chemistry (energetics)

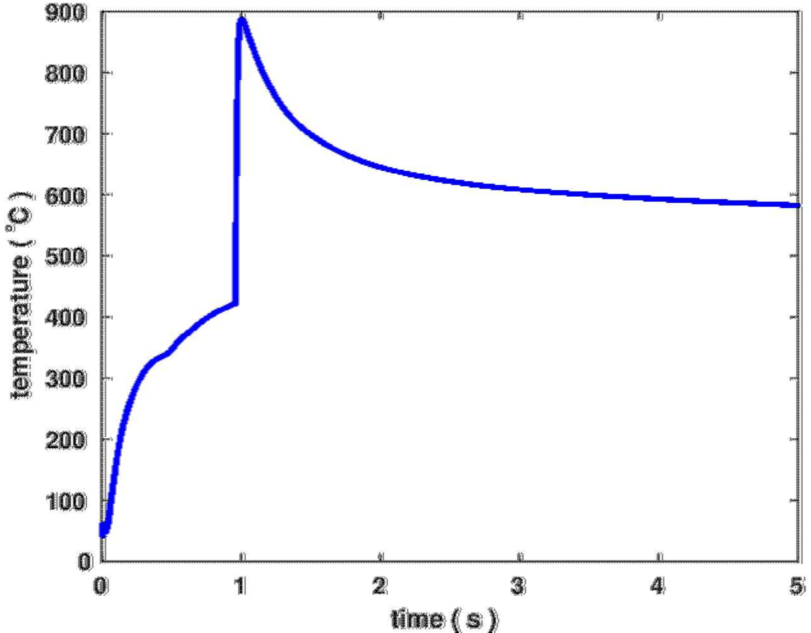
Backup

Thermally Activated Battery Simulator (TABS)

- Collection of software tools developed at Sandia over the last ten years to allow rapid assessment of thermal or electrochemical performance of a thermal battery design
- Full battery simulation of heat transfer
  - 2D axisymmetric
  - Captures heat generation and transport throughout the entire life of the battery (initiation, heat pellet burn, thermal diffusion, activation, heat loss through the case, and freeze out)
- Example of delayed battery initiation investigated by using TABS modeling to predict melting of electrolyte
- Also can show that delayed (auto) ignition of unfired heat pellet can lead to thermal runaway



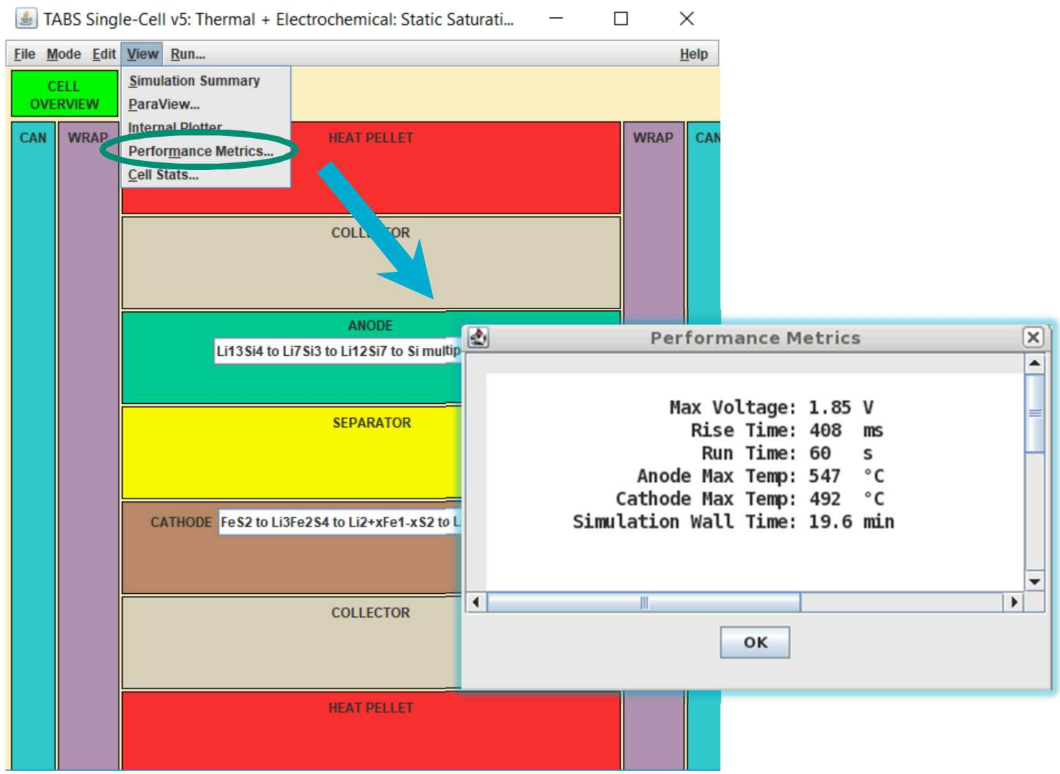




Thermally Activated Battery Simulator (TABS)

TABS
THERMALLY ACTIVATED BATTERY SIMULATOR

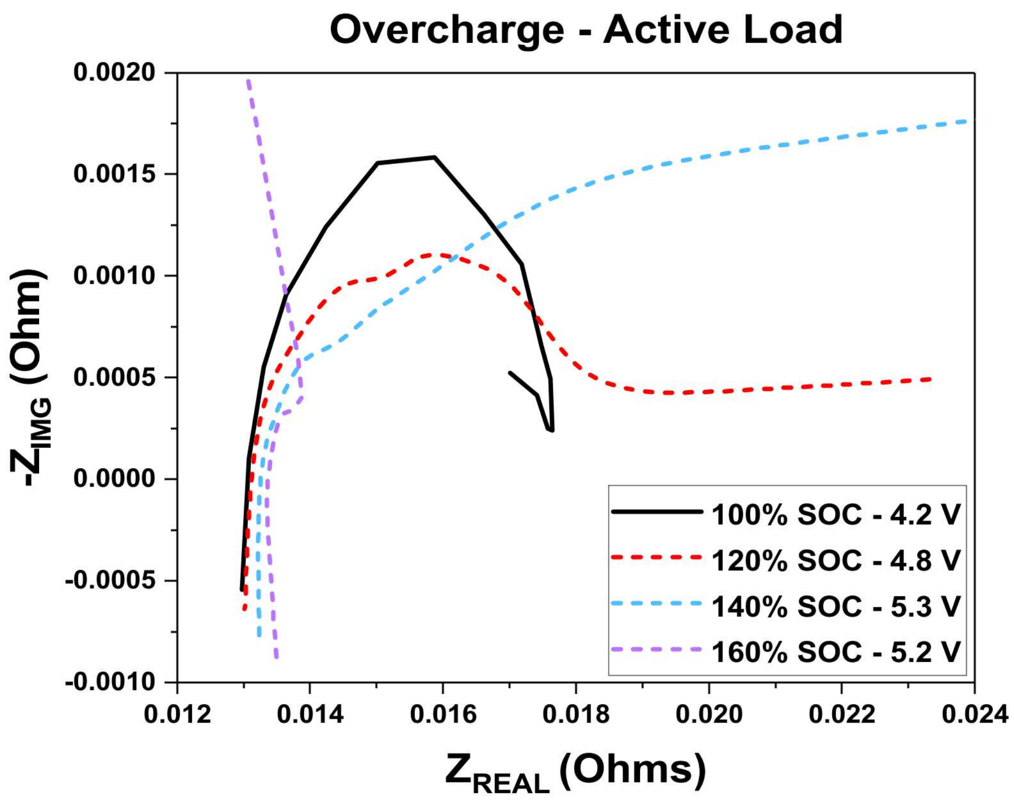
- Single cell simulation couples thermal, electrochemical and mechanical simulations
  - 1D electrochemical, 2D thermal, 2D thermal-electrochemical-mechanical
  - Predictive capability (voltage and current as a function of time)



Multiphysics simulations take into account heat transfer, phase change, mass transport, electrochemical performance and physical deformation during initiation, steady state operation and freeze out.

Fast Electrochemical Impedance Spectroscopy (EIS)

- 10s scan vs 10min+ for traditional EIS.
- Short scan time allows EIS monitoring during charge, including fast charge.
- Probe small systems (benchtop cells) for mechanistic studies, or scaled-up system for macroscopic effects. (commercial cells)
- Can be coupled with charge/discharge cycling to investigate phenomena *between* and *within* cycles.



Fast EIS under load (overcharge) , at Sandia