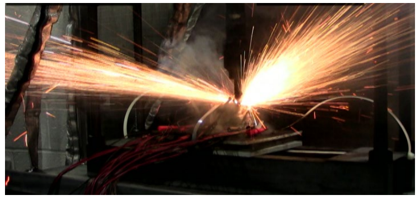
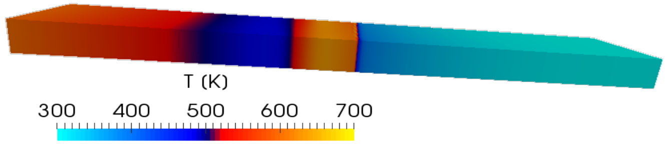
Predicting and Mitigating Cascading Failure in Stacks of Lithium-Ion Cells





PRESENTED BY

John Hewson, Andrew Kurzawski, Loraine Torres-Castro,

Randy Shurtz, Yuliya Preger, Joshua Lamb, Summer Ferreira

Office of Electricity Peer Review, September 23, 2019

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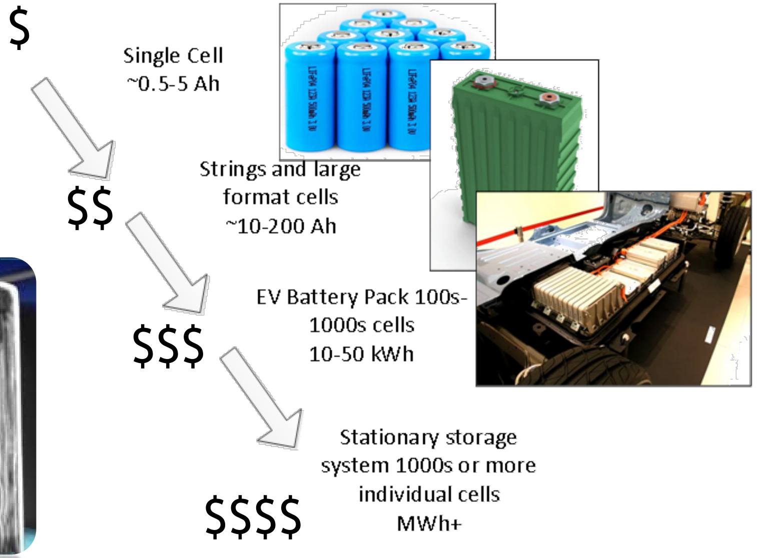
BACKGROUND OVERVIEW
Predicting and Mitigating Thermal Runaway

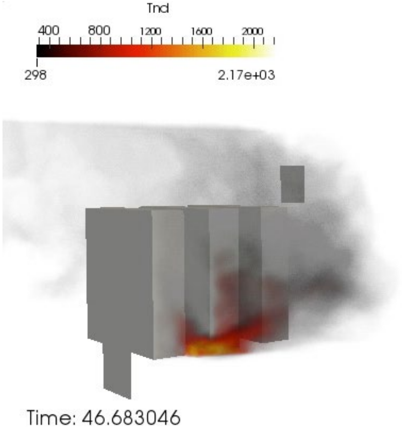
Validated safety and reliability is one of the critical challenges identified in 2013 Grid Energy Storage Strategic Plan

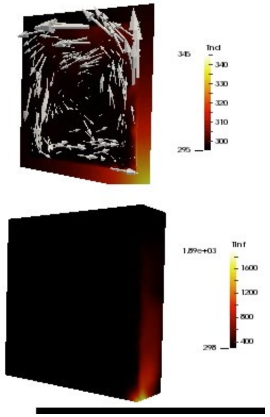


Safety incidents are rare but possible, including external causes.

How can we reduce facility investment risk?

- Prevent single point failure from cascading to large-scale system risk.
- Current approach is test to safety.





Large-scale testing is costly and simulations allow exploration of the design space if well grounded in reality.

- Link source terms to material science – tomorrow Randy Shurtz talk.

www.cnn.com
www.samsung.com
www.internationalbattery.com
www.nissan.com
www.saft.com

OVERVIEW
Predicting and Mitigating Thermal Runaway

How can we reduce facility investment risk?

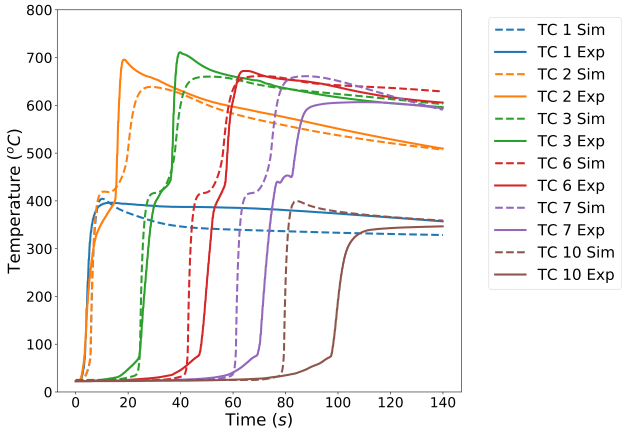
- Identify boundaries between mitigation and cascading failure

Short circuit simulated in first cell acts as boundary condition

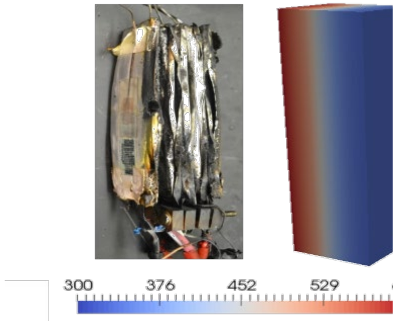
Lamb, J., et al. (2015). J. Power Sourc

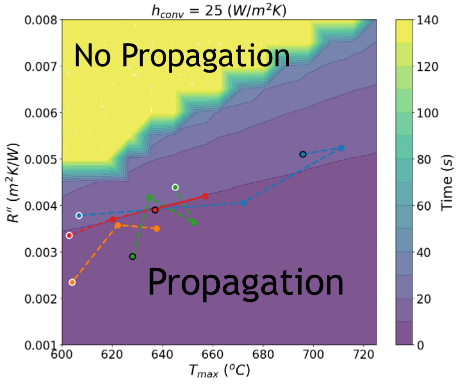
OBJECTIVES
Predicting and Mitigating Thermal Runaway

Validated safety and reliability is one of the critical challenges identified in 2013 Grid Energy Storage Strategic Plan



1. ***Develop validated predictive models of cell-to-cell*** then module-to-module propagation.
   - Concurrent ***experimental program*** for validation (Loraine Torres-Castro)
   - Other tasks link predictive heat release to material science (Randy Shurtz)
2. Identify ***boundaries of propagation versus mitigation***
   - ***Thermal aspects of system design***
   - Electrical aspects of system design
   - Battery chemistry and material science
   - Algorithms for active control strategies.
3. Develop capabilities to evaluate design tradeoffs.
4. Promote a broader acceptance of quality approaches to energy storage safety.





METRICS AND MILESTONES

Predicting and Mitigating Thermal Runaway

MILESTONES

- Relate material models to experimental measurements at multi-cell level.
- Address safety modeling associated with thermal modifications. Determine limits of cascading failure.
- Future goals listed on Looking Forward slide.

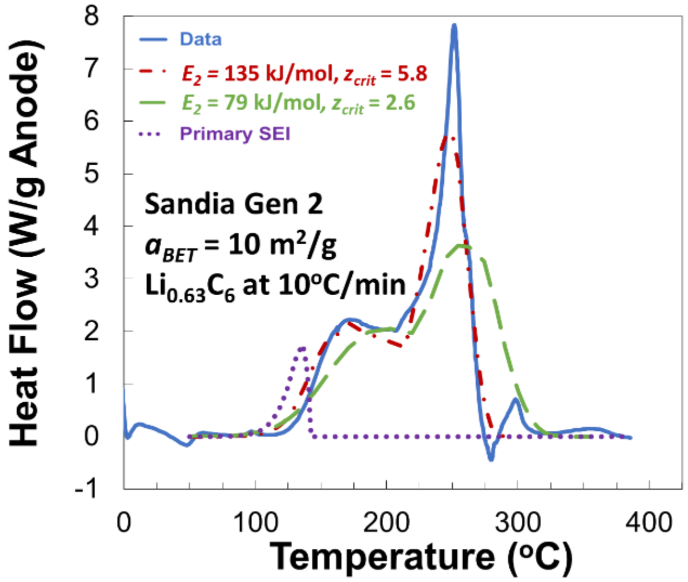
RESULTS

- Implement new high-temperature chemistry according to statistical analysis of calorimetry and propagation.
- Provides ***factor of two global improvements*** in propagation predictions.
- Increased heat capacity per stored energy mitigates propagation.
- Thermal resistance between cells contributes. Mapped out limits.
- ***Quantified relative effectiveness*** experimentally and through predictions.

CHALLENGES

Most models for thermal runaway heat sources are ~20 years old

- Successful in terms of single-cell onset
- Lack higher-temperature measurements needed for cascading failure prediction.
- Lack tie to material science developments.
- 2018 addressed anode heat release models



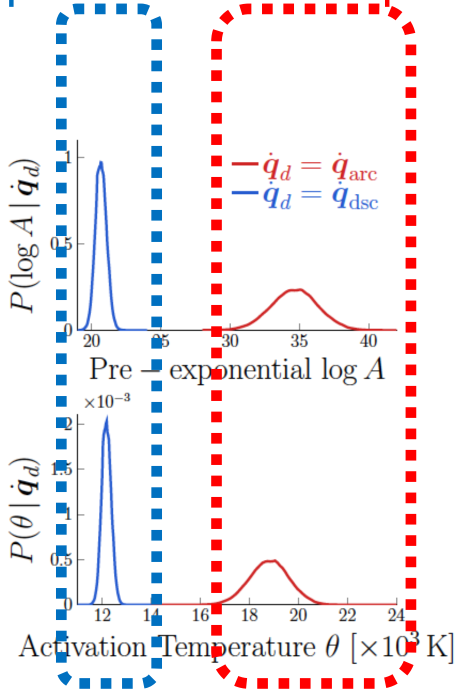
RESULTS Predicting and Mitigating Thermal Runaway

CHALLENGE: No measurements of thermochemical decomposition rates at propagation temperatures.

- Bayesian analysis of cathode runaway calorimetry measurements:
  - ARC and DSC measurements show two distinct parameter sets.
  - Both consistent within expt. uncertainty.
  - Suggests adjustments in high-temp chemistry/ physics giving improved predictions.
- See also Randy Shurtz talk on cathode chemistry tied to new materials

Bayesian likelihood of cathode rate parameters

DSC parameters ARC parameters



RESULTS - Predicting and Mitigating Thermal Runaway

Cascading failure testing with thermal inserts: metallic spacers between cells

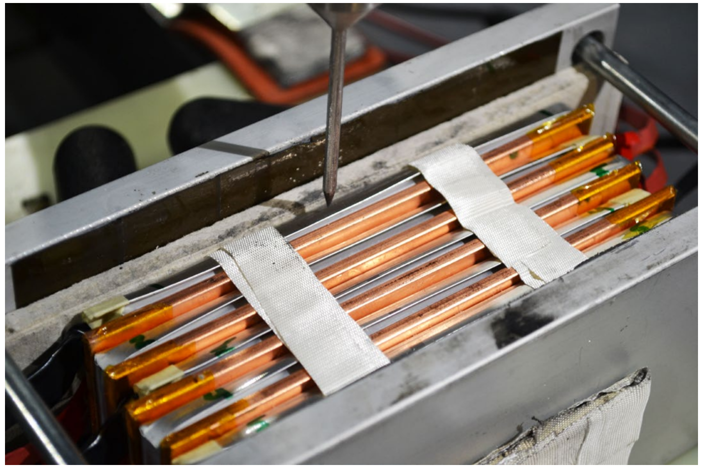
$LiCoO_2$ 3Ah pouch cells

5 closely packed cells with/without aluminum or copper spacer plates

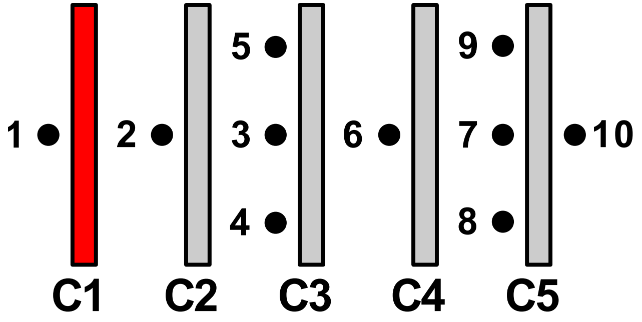
- Spacer thicknesses between 1/32" and 1/8"
- State of charge between 50% and 100%

Failure initiated by a mechanical nail penetration in the outer cell (cell 1)

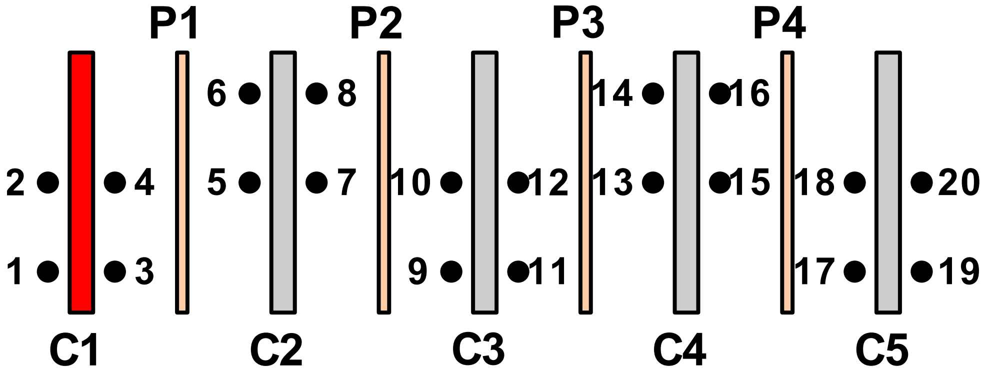
Thermocouples (TC) between cells and spacers (if present)



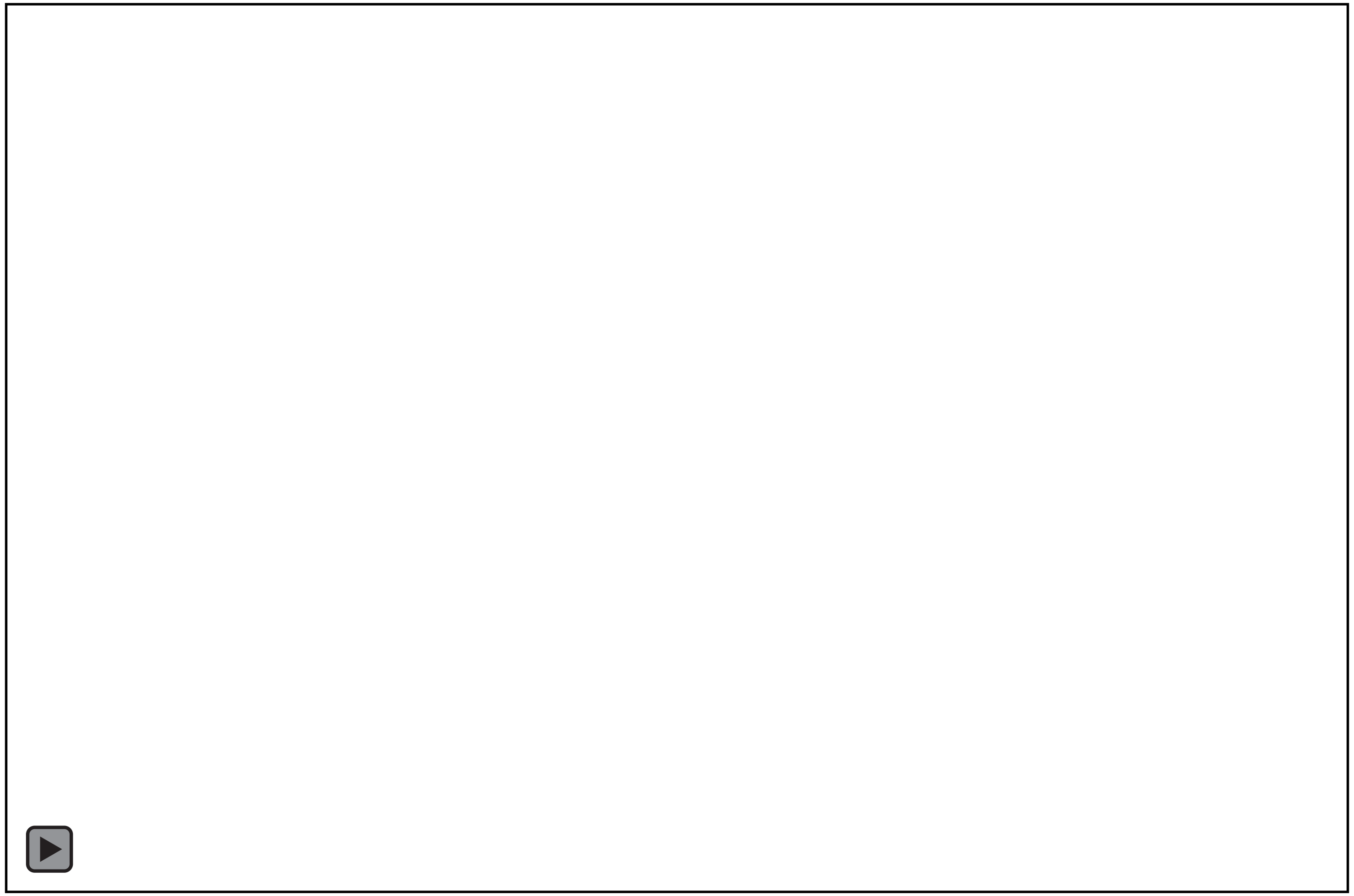
Thermocouple Locations



Thermocouple Locations with spacer plates

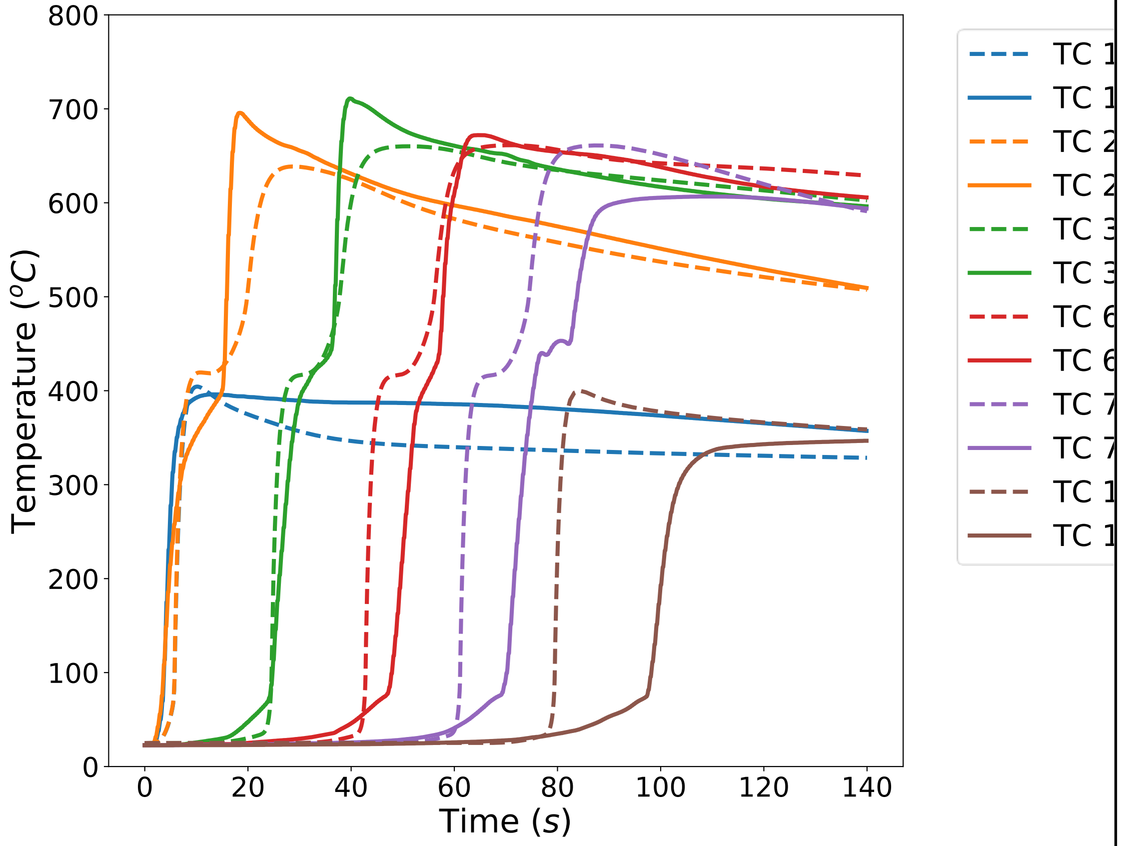


Cascading failure testing



RESULTS - Predicting and Mitigating Thermal Runaway

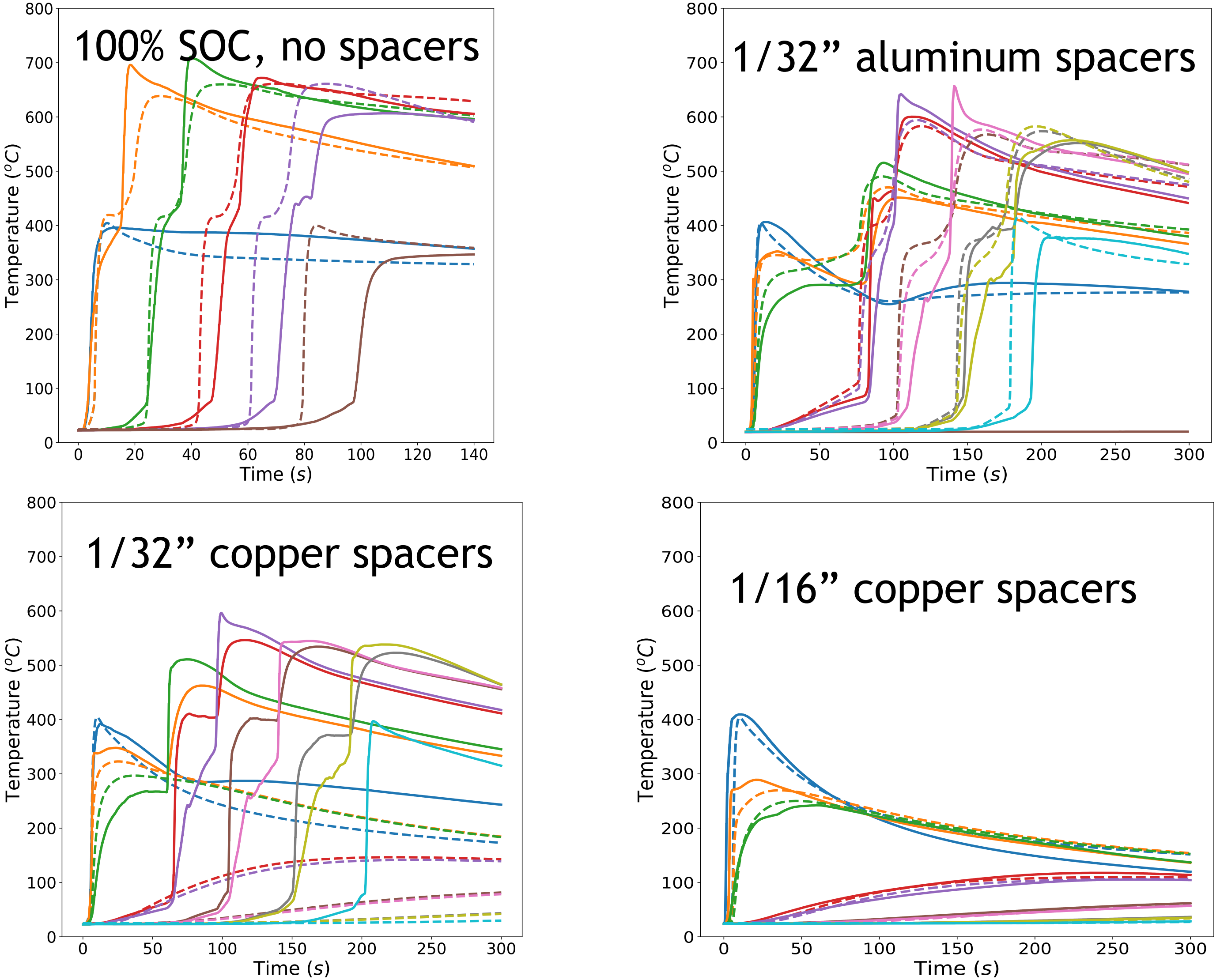
Simulation and measurements: 100% SOC, no



- Prediction of peak temperatures and cooling
- Cell crossing speed over-predicted

RESULTS - Predicting and Mitigating Thermal Runaway

Temperature-time propagation measurements and predictions



Metallic inserts

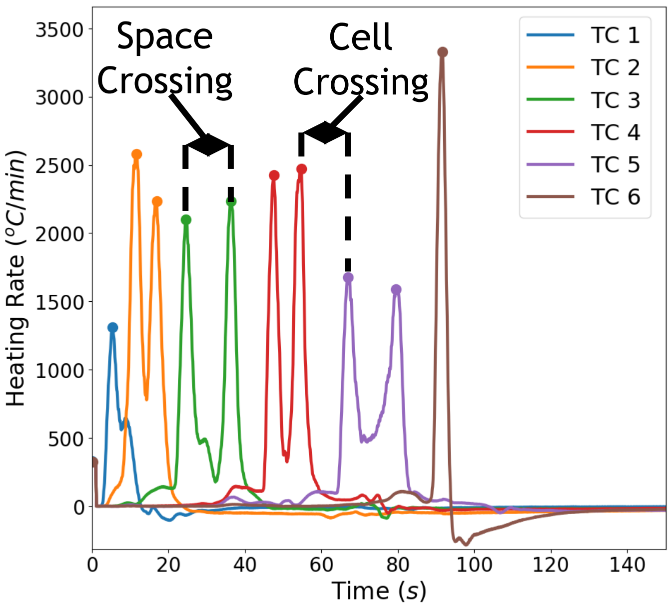
- Add heat capacity.
- Increase time delay for cell runaway.
- Prevent propagation for 30% increase in net heat capacity.
- Reduced SOC results suggest homogeneous heat capacity changes of 25% sufficient.

- Simulations more sensitive to mitigation than observation.

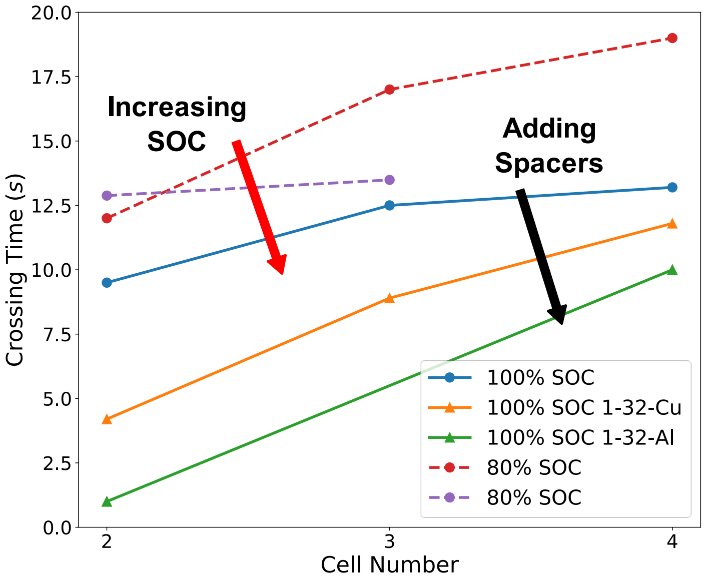
RESULTS - Predicting and Mitigating Thermal Runaway

Cascading failure propagation rates.
Global rates allow estimates of possible active cooling requirements.

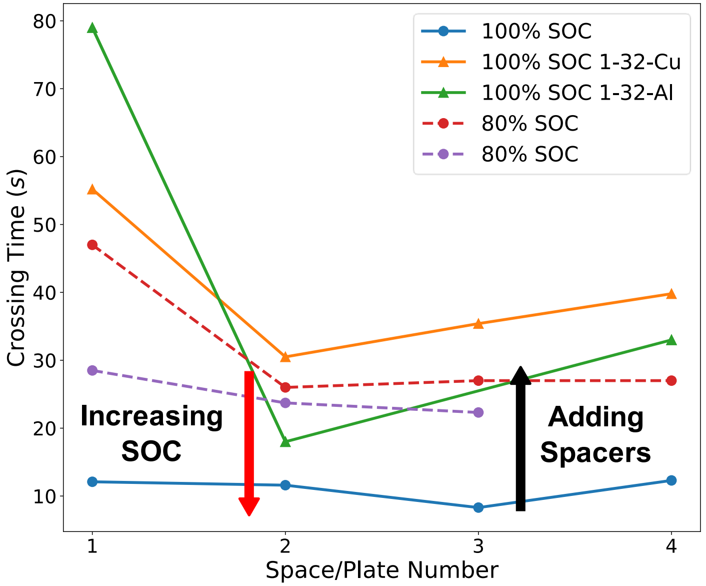
Thermocouple time derivatives



Cell-crossing time



Space/gap-crossing time



Adding spacers **increases** space crossing time, but **decreases** cell crossing time.

Increasing state of charge (SOC) decreases both space and cell crossing time.

RESULTS - Predicting and Mitigating Thermal Runaway

Heat capacity and SOC propagation/mitigation summary

Quantified: Increased heat capacity per stored energy can inhibit cascading propagation.

State of Charge	Experiment	Simulation
100% SOC	Propagation	Propagation
90% SOC	N/A	Propagation
80% SOC	Propagation	No Propagation
75% SOC	No Propagation	No Propagation

Results suggest homogeneously distributed heat capacity is more effective than intermittent heat sinks.

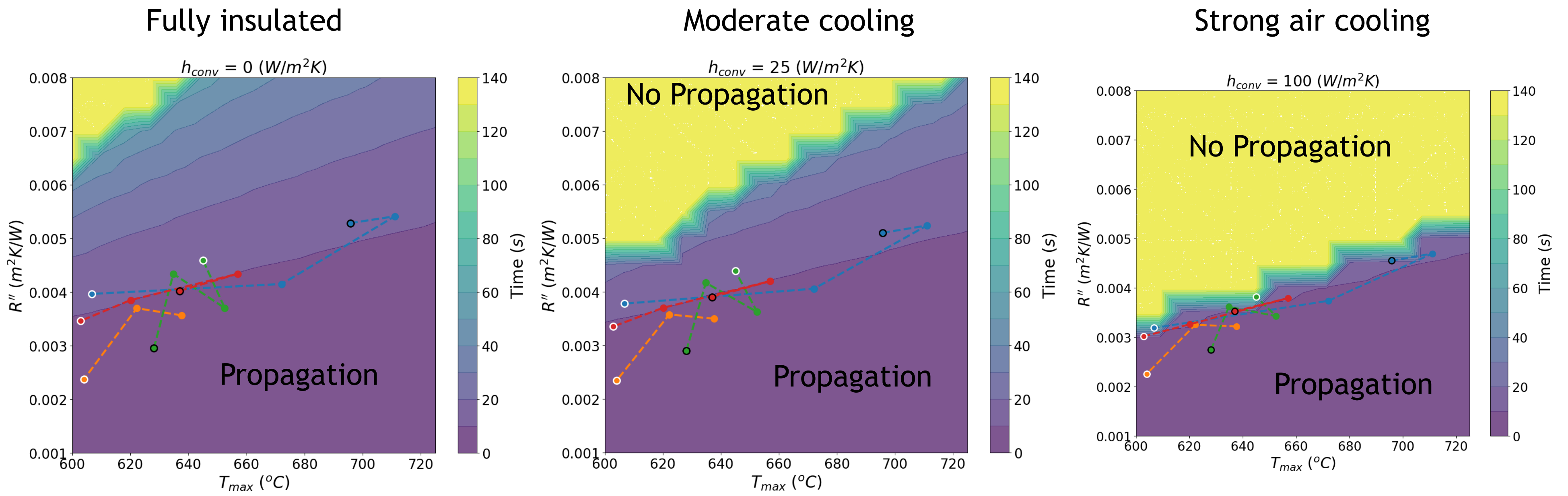
Effective Heat Capacity	Experiment	Simulation
778 J/kg/K (no spacers)	Propagation	Propagation
893 J/kg/K (1/32" Al)	Propagation	Propagation
941 J/kg/K (1/32" Cu)	Propagation	No Propagation
1009 J/kg/K (1/16" Al)	No Propagation (Cell 2 Failure)	No Propagation
1103 J/kg/K (1/16" Cu)	No Propagation (Cell 2 Failure)	No Propagation

RESULTS - Predicting and Mitigating Thermal Runaway

Limits of cascading thermal runaway

Energy per heat capacity, cooling and inter-cell resistance defines propagation limits

Model maps delay in propagation: yellow region is infinite delay—*failure to propagate*.



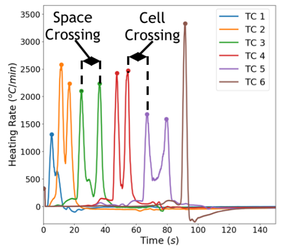
Convection cooling and conduction through stack results in failure to propagate for some scenarios.

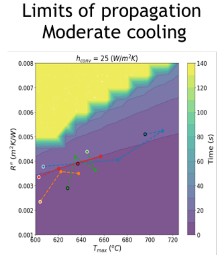
Consider cost/design tradeoff : cooling versus thermal resistance.

LOOKING FORWARD

From defining limits of propagation at cell-stack level to larger-scale facilities:

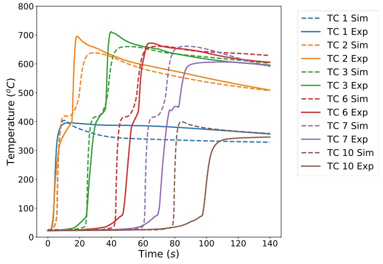
- Module and rack-scale heat release and dissipation.
- Improved thermal source term models for new battery materials.





Developing open-source application to analyze thermal-runaway mitigation designs

- Stand-alone application to analyze cell-stack and eventually module-scale then rack-scale scenarios.
- Analyze consequences of various abuse scenarios.
- Develop robust mitigation approaches to fit your economic model.



Cell venting of flammable gases: Flammability and heat release consequences.

- Flammability of unignited mixtures: CO-H2 versus electrolytes.
- Heat release distribution, consequences and dissipation.

LOOKING FORWARD

Collaborative workshops: Thermal Runaway Investigation, Prediction and Prevention

- Follow models of *Turbulent Nonpremixed Flames Workshop* (https://www.sandia.gov/TNF/abstract.html), *Measurements and Computation of Fire Phenomena Workshop* (https://iafss.org/macfp/)
- Setup online forum for validation quality measurements and validated predictive models.
- Collaboratively address inconsistencies across literature.
- Organizational meeting at Dallas ECS meeting, May 2019 including range of contributing institutions.
- *J. Electrochem. Soc.* Perspectives paper on calorimetry measurements. Difficult to predict broadly across different systems.

Suggest ***collaborative workshop*** structure ***bringing together experimentalists and modelers*** to create a ***dialogue*** working through these challenges.

PUBLICATIONS AND PRESENTATIONS

Publications

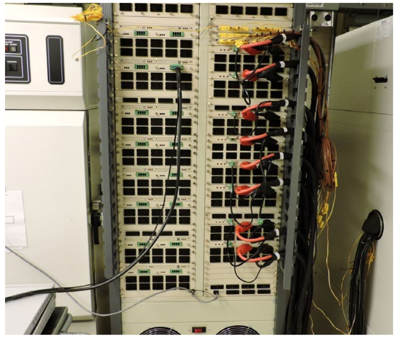
- R. C. Shurtz, Y. Preger, L. Torres-Castro, J. Lamb, J. C. Hewson and S. Ferreira, "**Perspective—From Calorimetry Measurements to Furthering Mechanistic Understanding and Control of Thermal Abuse in Lithium-Ion Cells,**" *J. Electrochem. Soc.*, 166, A2498, 2019
- R. C. Shurtz, J. D. Engerer and J. C. Hewson, "**Predicting High-Temperature Decomposition of Lithiated Graphite: Part I. Review of Phenomena and a Comprehensive Model**," *J. Electrochem. Soc.*, 165, A3878 (2018). DOI 10.1149/2.0171814jes
- R. C. Shurtz, J. D. Engerer and J. C. Hewson, "**Predicting High-Temperature Decomposition of Lithiated Graphite: Part II. Passivation Layer Evolution and the Role of Surface Area,**" *J. Electrochem. Soc.*, 165, A3878 (2018). DOI 10.1149/2.0171814jes
- **Mitigation of Failure Propagation in Multi-Cell Lithium Ion Batteries** (in preparation)

Presentations and Proceedings

- **Toward understanding and preventing cascading failure with computer modeling**; *ESS Safety Workshop*, Albuquerque, March 2019.
- **Predicting and Mitigating Cascading Failure of Thermal Runaway in Stacks of Li-Ion Pouch Cells,** *11th FM Global Open Source CFD Fire Modeling Workshop*, Norwood, MA, June 2019.
- A. Kurzawski, R. Shurtz, L. Torres-Castro, J. Lamb, and J. C. Hewson, "**Predicting Limits of Cascading Failure of Thermal Runaway in Stacks of Li-Ion Pouch Cells**," *Proc. Western States Section Combust. Instit.*, October 2019.

TEAM Predicting and Mitigating Thermal Runaway

Sandia Battery Test Facilities

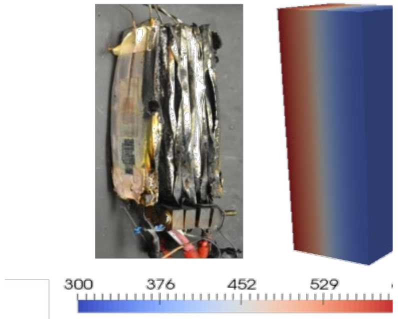


Summer Ferreira
Yuliya Preger
Armando Fresquez
Heather Barkholtz (former SNL)

Sandia Battery Abuse Lab

Loraine Torres-Castro
Joshua Lamb
Jill Langendorf

Sandia Fire Sciences



John Hewson
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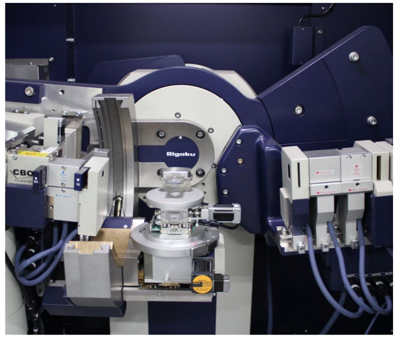
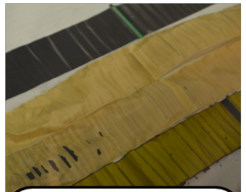
Center for Integrated Nanotechnologies



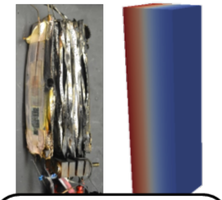
Sergei Ivanov

Baseline electrochemical performance analysis

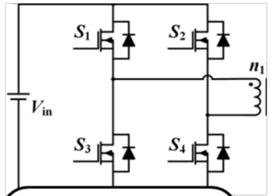


Materials characterization and thermal stability testing

Whole-cell abuse response analysis



Modeling of thermal propagation

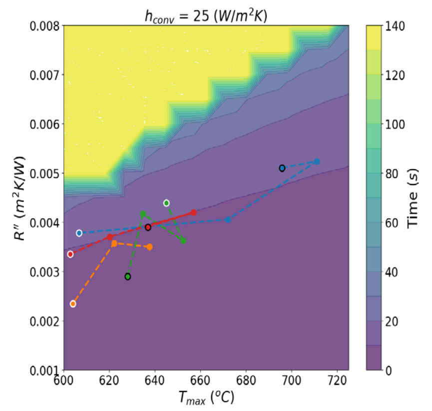


Design of new power electronics for battery safety

SUMMARY

- Thermal runaway is a risk and potential barrier to development and acceptance.
- Multi-physics thermal models are identifying critical ignition and propagation trends.
- Quantifying mitigation strategies in terms of physical parameters.
- Progress this term
  - Bayesian analysis of cathode measurements show parameter range allowing improved propagation predictions.
  - Predictions and measurements of cell-to-cell propagation with varying SOC and thermal mitigation.
  - Identify cascading failure limits: heat release per heat capacity (homogeneous and inhomogeneous) -- combine with last-year's analysis of thermal resistance.

Limits of propagation
Moderate cooling



Thank you

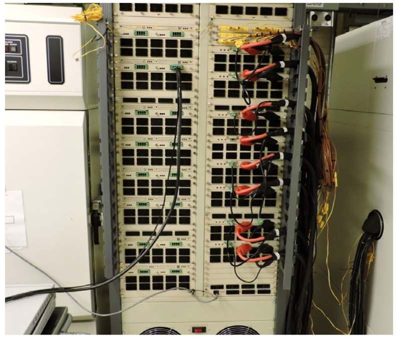
- Funded by the U.S. Department of Energy, Office of Electricity, Energy Storage program under the guidance of Dr. Imre Gyuk, Program Director.

- Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525.

- For further information: John Hewson - jchewso@sandia.gov

Reviewer Slides Project team

Sandia Battery Test Facilities



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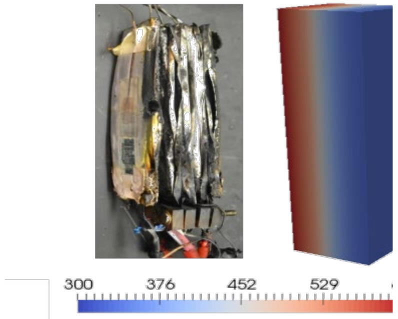

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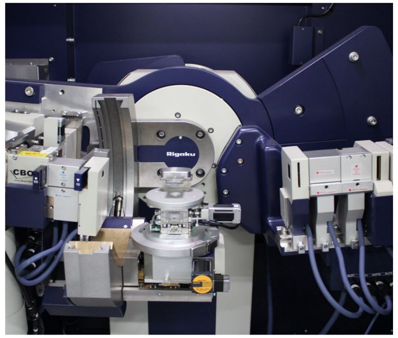

Sergei Ivanov

This Sandia program brings together core capabilities in

- Thermal abuse of battery systems through Battery Abuse Lab.
- Fire hazard analysis for energy-containing system through the fire science based nuclear deterrent safety.
- High temperature chemistry and reacting systems through the Combustion Research Facility.