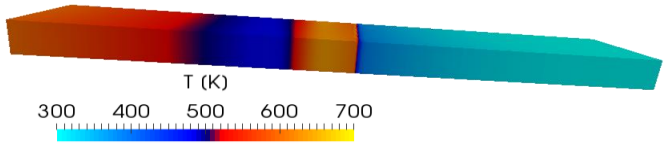
Thermal Analysis to Mitigate Cascading Propagation of Lithium-Ion Cell Stacks



PRESENTED BY

John Hewson, Andrew Kurzawski, Randy Shurtz,

Loraine Torres-Castro, Yuliya Preger, Joshua Lamb

Office of Electricity Peer Review, September 30, 2020

SAND2020-10222 C

SAND2019-11411 C

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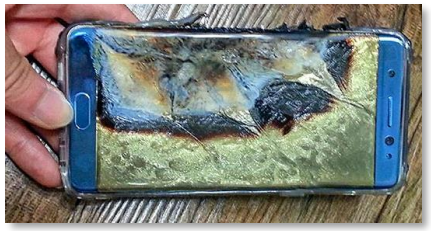
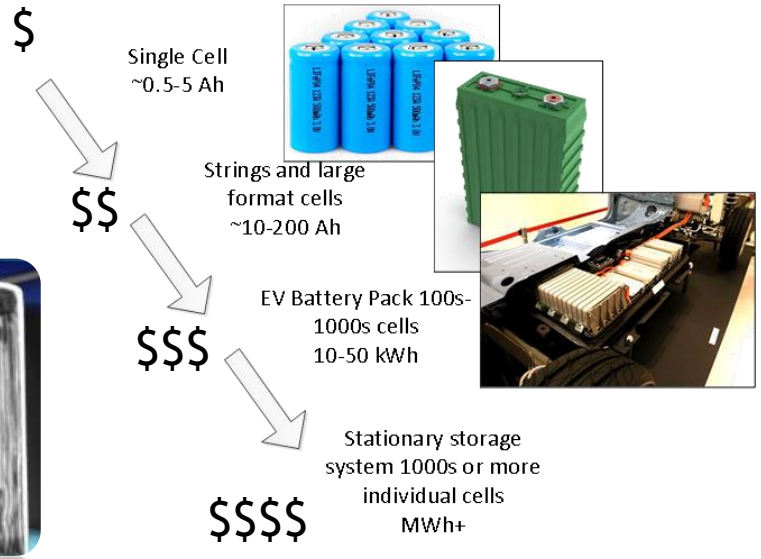
BACKGROUND OVERVIEW
Predicting and Mitigating Thermal Runaway



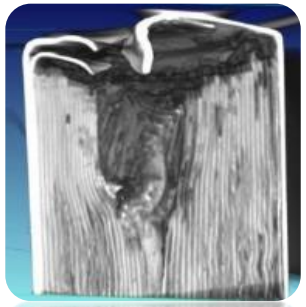
Validated safety and reliability is one of the critical challenges identified in 2013 Grid Energy Storage Strategic Plan

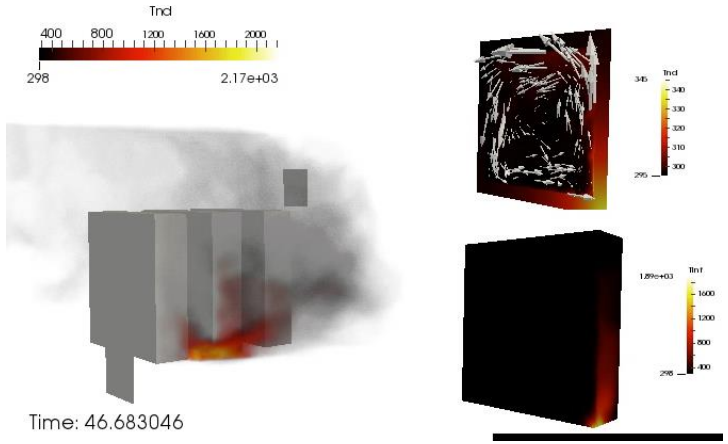


Safety incidents are rare but possible, including external causes.

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.

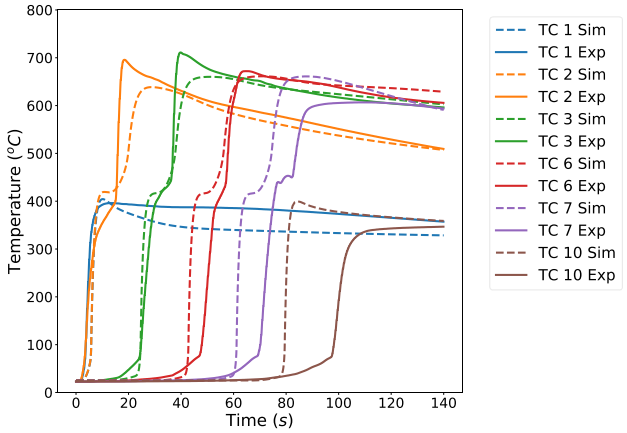
- We link source terms to material science – morning talk by Randy Shurtz.

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

OBJECTIVES

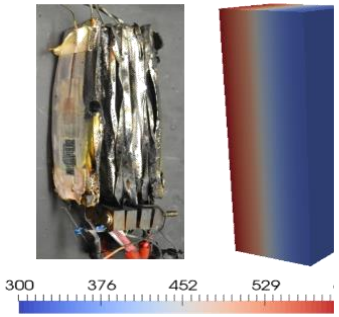
Provide robust system scale safety and reliability

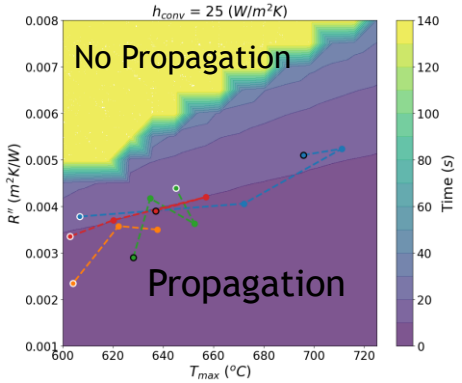
Validated safety and reliability is one of the critical challenges identified in 2013 Grid Energy Storage Strategic Plan



Develop methods to mitigate point failures and avoid propagation

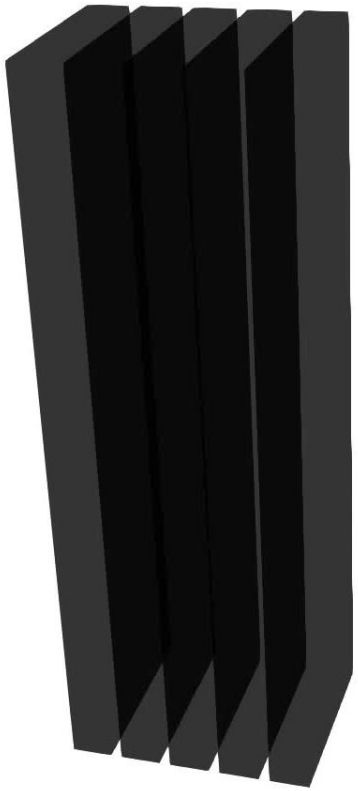
1. **Develop validated predictive models of cell-to-cell** then module-to-module propagation.
   - Concurrent **experimental program** for validation (Loraine Torres-Castro)
   - Other tasks link predictive heat release to material science (Randy Shurtz)
2. Identify **boundaries of propagation versus 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.

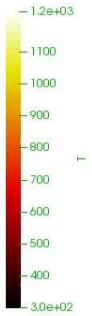




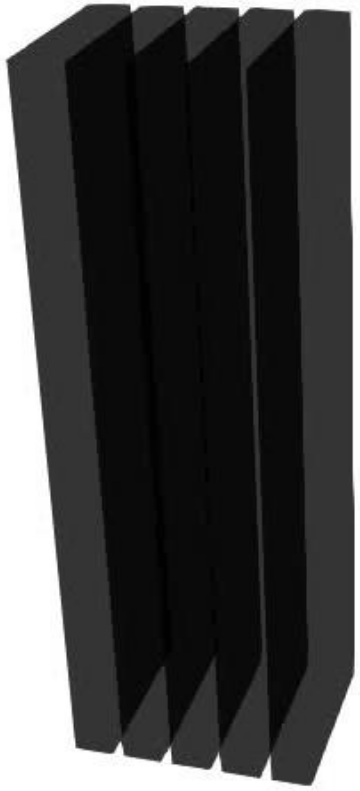
OVERVIEW – Reduce facility investment risk: Identify boundaries between mitigation and cascading failure

Short circuit simulated in first cell acts as boundary condition →





Baseline cell stack: Thermal runaway propagates

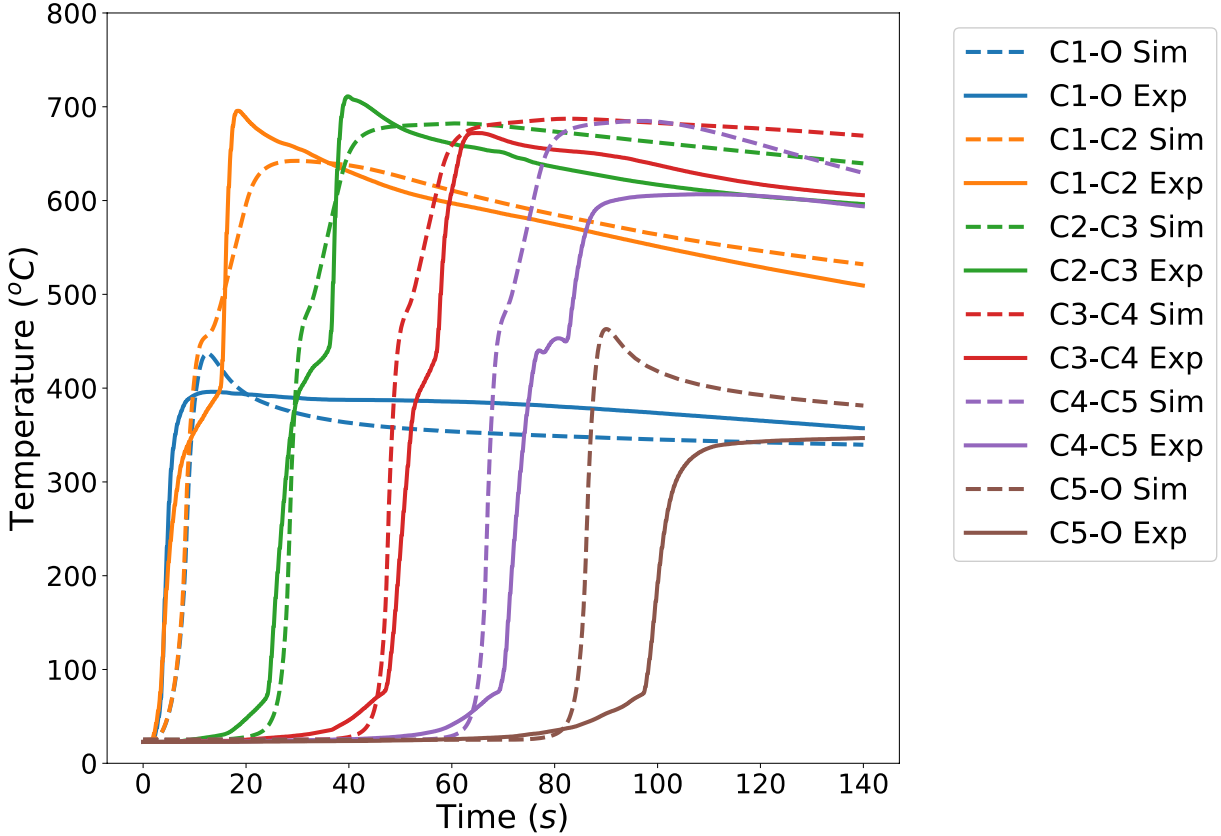


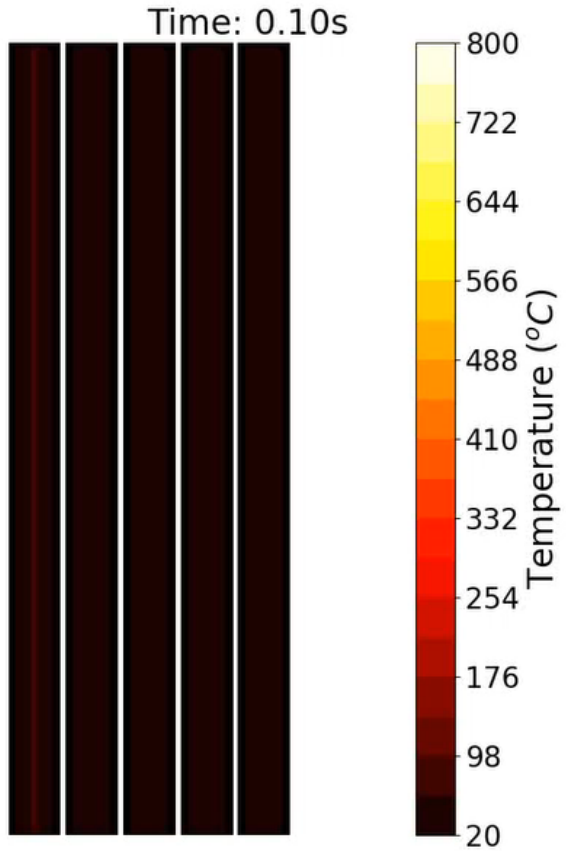
Thermal modifications (Reduced conductivity, increased contact resistance): **Propagation mitigated.**

Torres-Castro, L. et al., (2020) J Electrochem. Soc., **167**(9): 090515
Lamb, J., et al. (2015). J. Power Sources **283**: 517-523.

RESULTS - Predicting Thermal Runaway

Simulation and measurements: 5 x 3 Ah LCO cells, 100% SOC, no plates



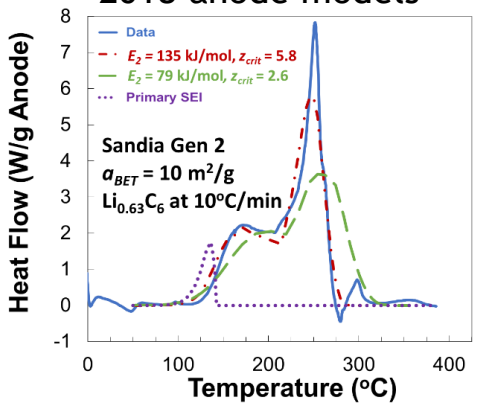


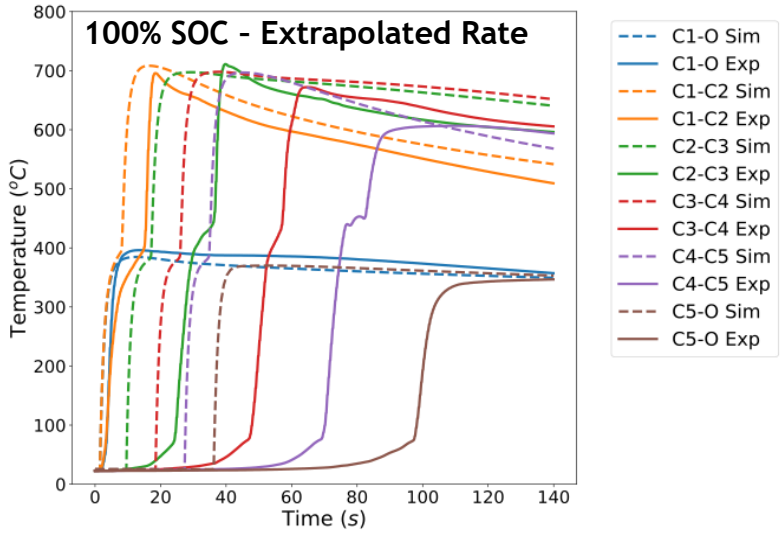
RESULTS - Predicting Thermal Runaway

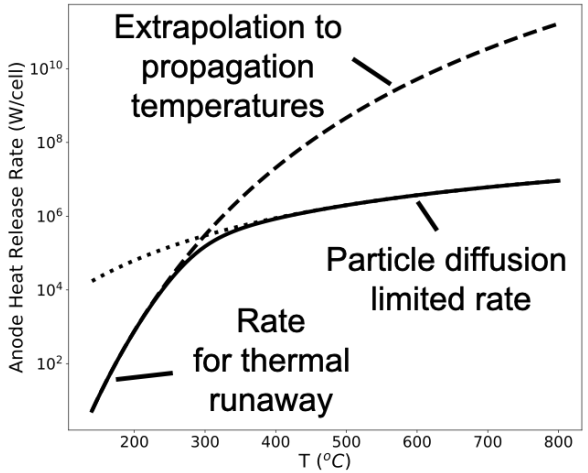
Challenge: Calorimetry measurements only at lower temperatures.

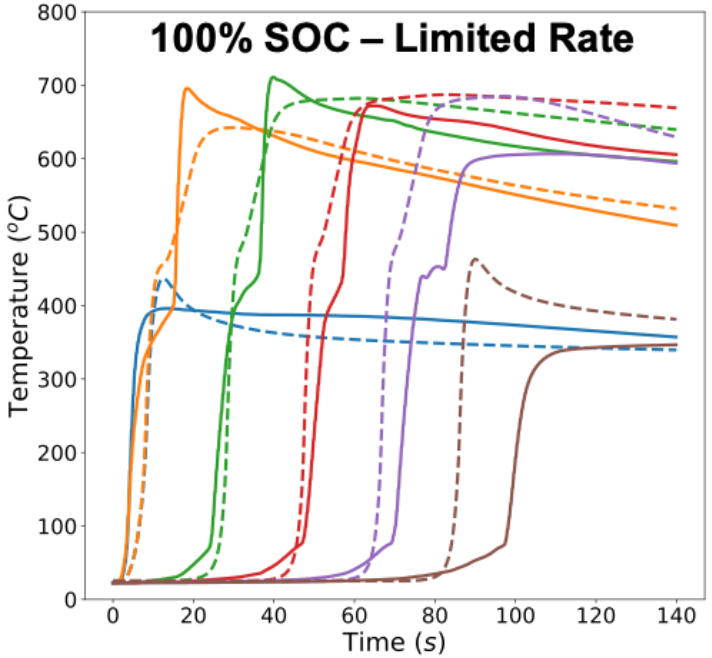
- Extrapolating thermal runaway models to cascading failure predicts too-fast propagation.
- Lack higher-temp measurements to predict cascading failure.

2018 anode models









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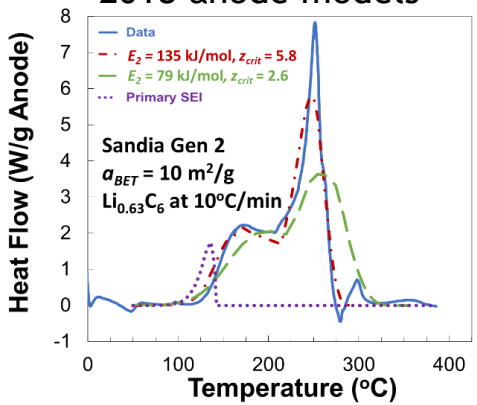

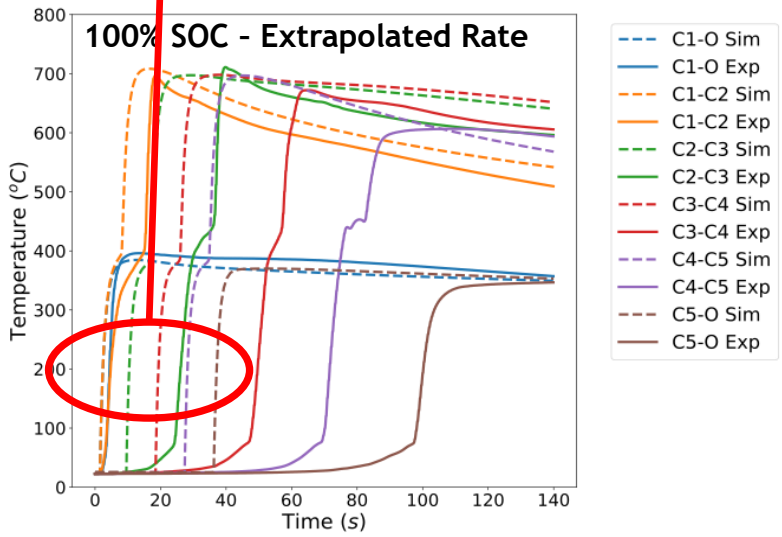

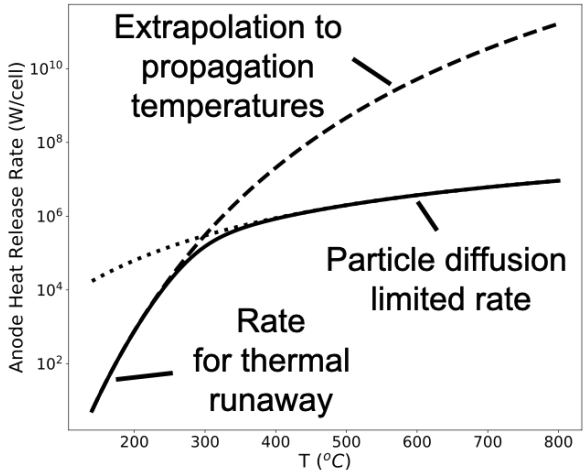

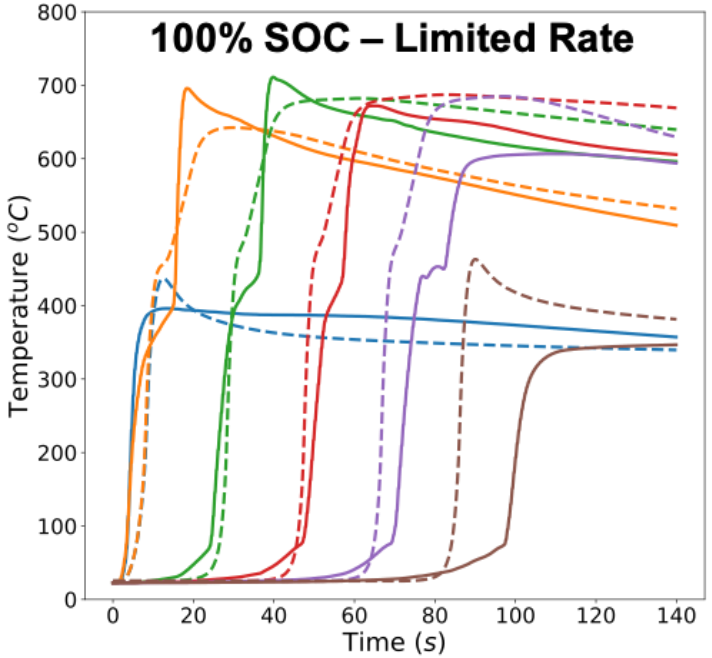

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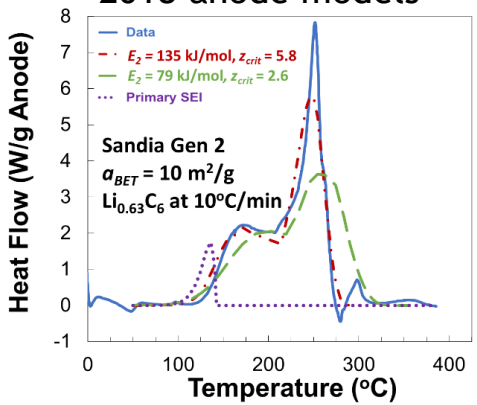

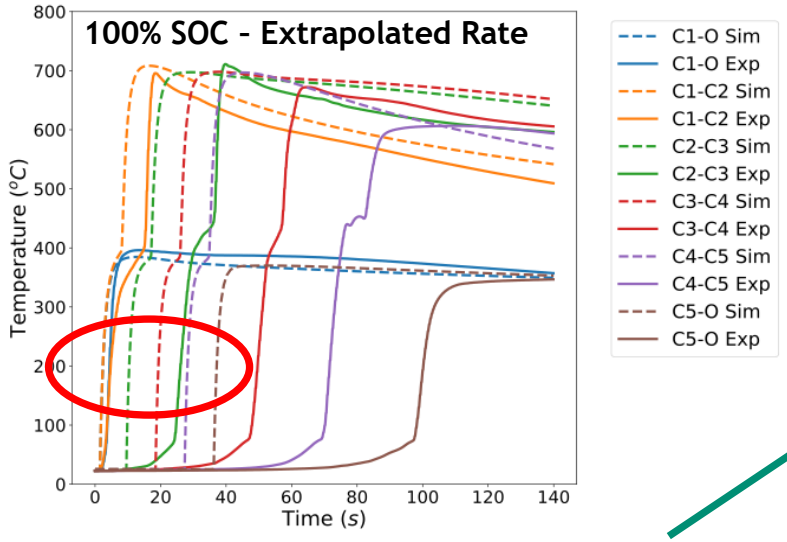

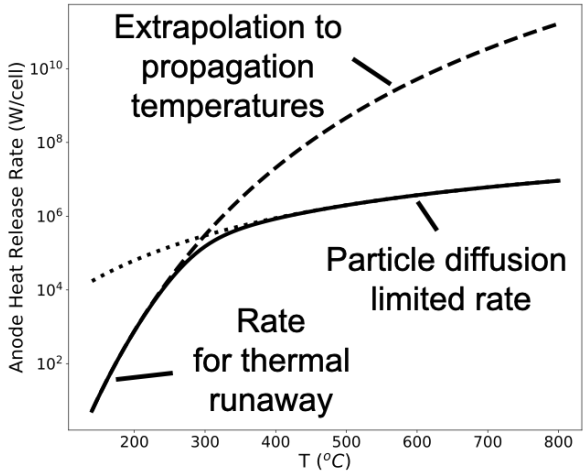

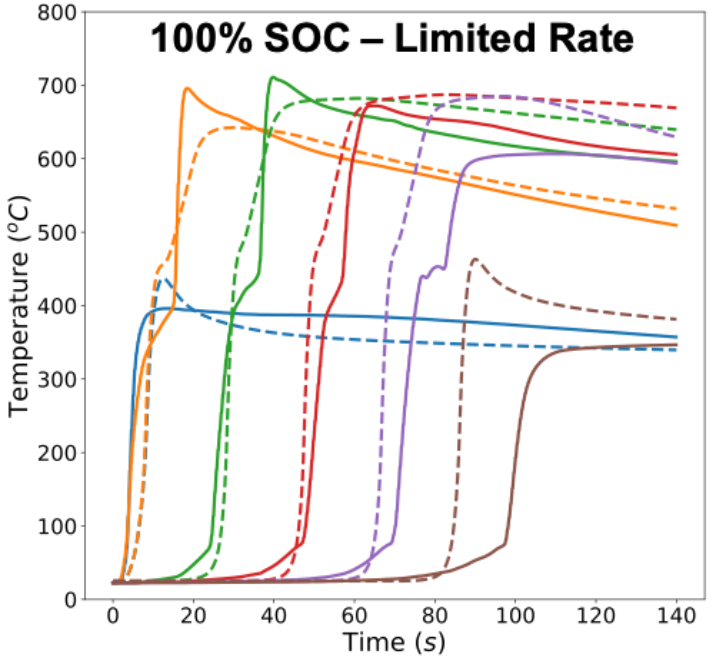

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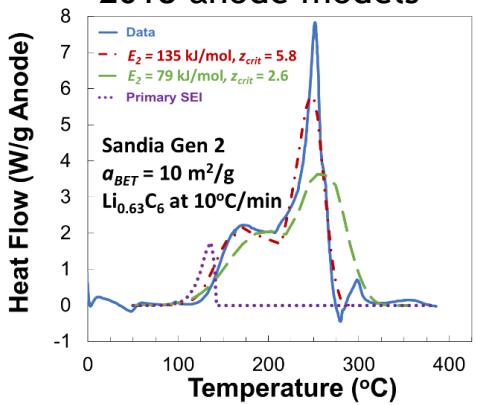

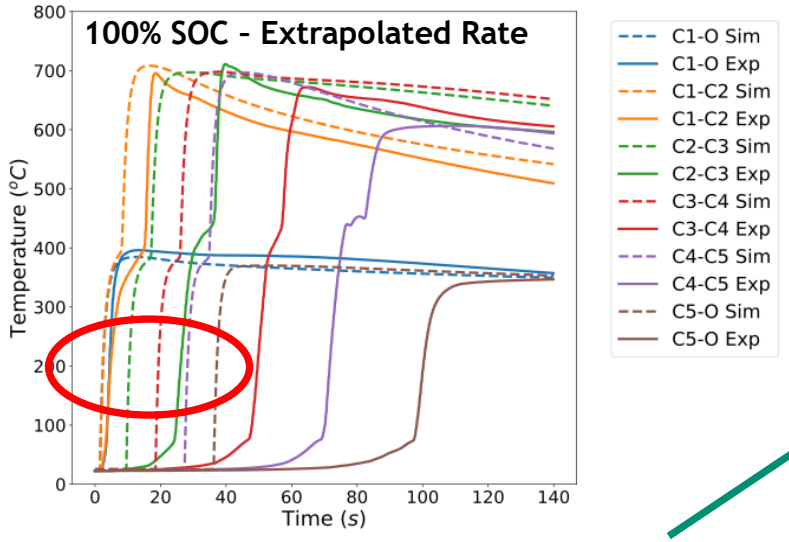

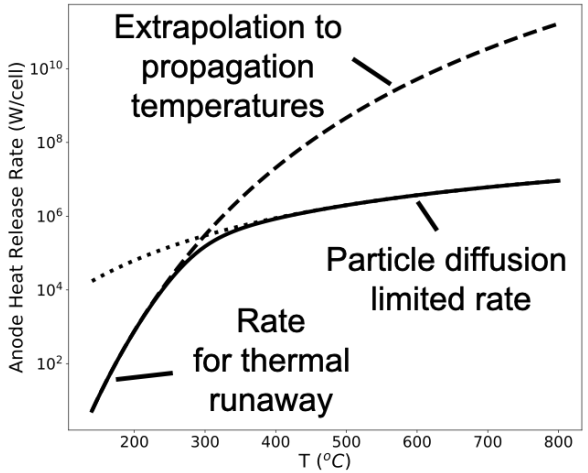

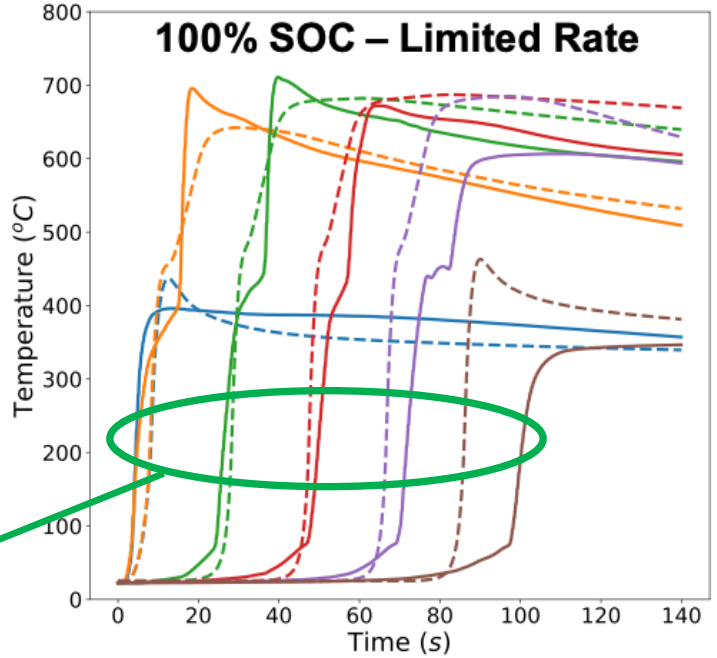

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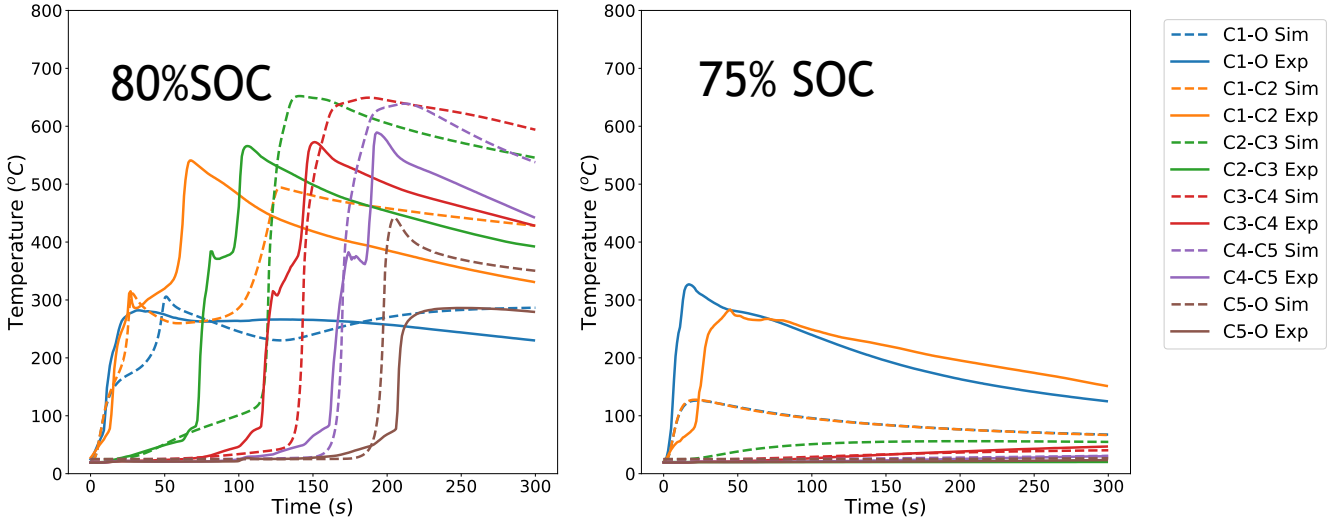
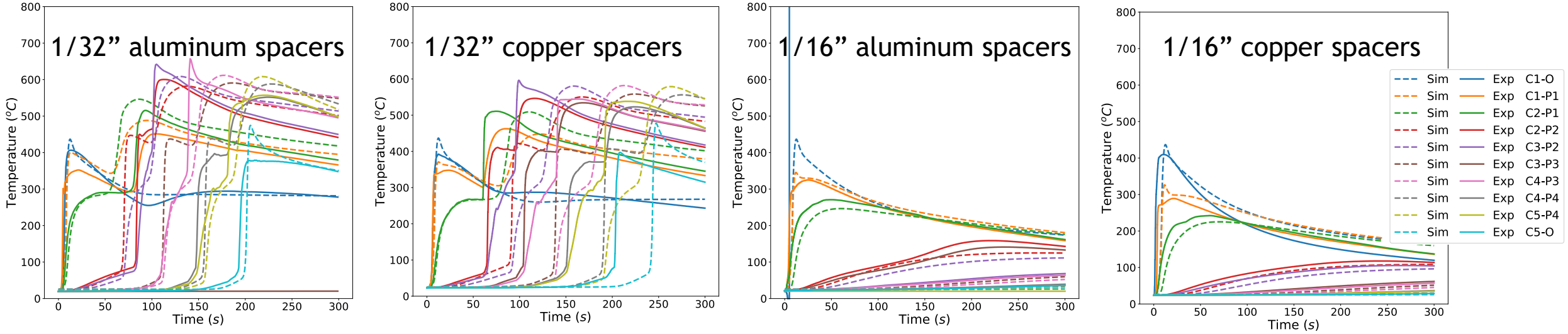
RESULTS - Predicting Thermal Runaway Propagation/Mitigation

Temperature-time propagation measurements and predictions



- Successful prediction over a range of reduced SOC and metallic inserts.
- Collectively add heat capacity & increase time delay for cell runaway.
- Prevent propagation for 30% increase in net heat capacity.



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RESULTS - Predicting Thermal Runaway Propagation/Mitigation

Heat capacity/plates and SOC propagation/mitigation summary

State of Charge	Experiment	Simulation
100% SOC	Propagation	Propagation
80% SOC	50/50 Propagation	Propagation
75% SOC	No Propagation	No Propagation
50% SOC	No Propagation	No Propagation

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	Propagation
1009 J/kg/K (1/16” Al)	No Propagation	No Propagation
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Quantified: Increased heat capacity per stored energy can inhibit cascading propagation.

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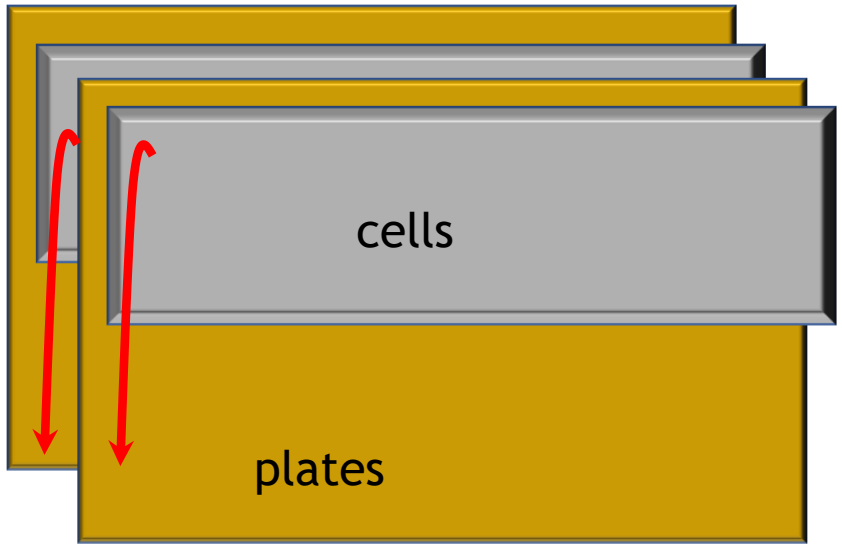
Can we use thin plates to dissipate heat to the rest of the structure/cooling system?



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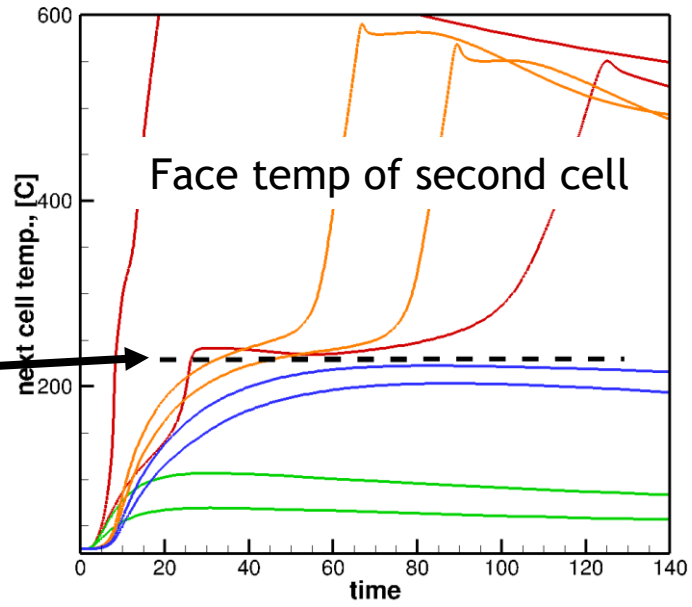
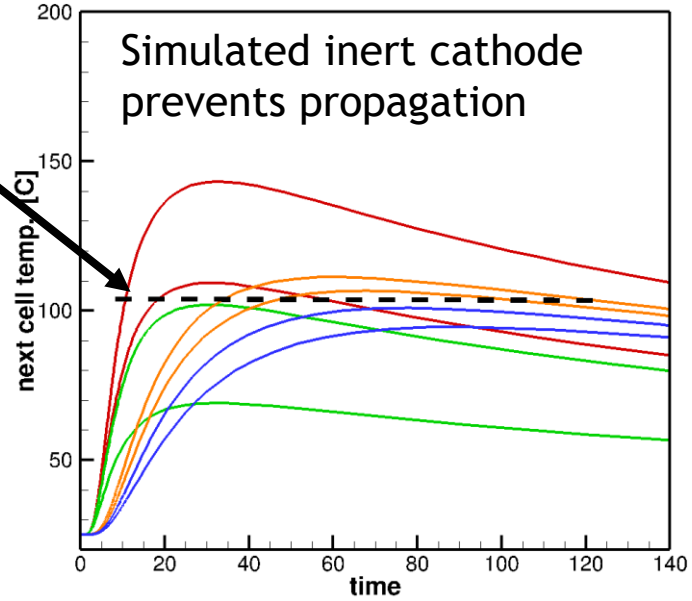
RESULTS – Opportunities with Predictive Simulations

Demonstrated predictive capabilities allow us to ask design questions about previous cases:

- What cell temperature must be avoided to prevent propagation?
  - Next-cell face temperature shows limiting value.
    Warm colors propagation; cool colors mitigation
  - Cleaner separation if we simulate inert cathode.
- Also note time delay with plates versus no plates.





- Time delays are opportunities to dissipate heat.
- *But time to conduct heat along plate is long: (20-30 s)*

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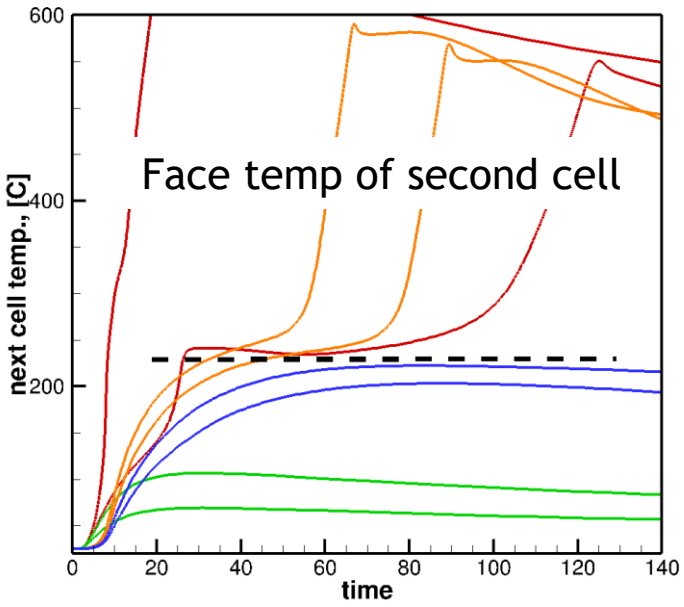

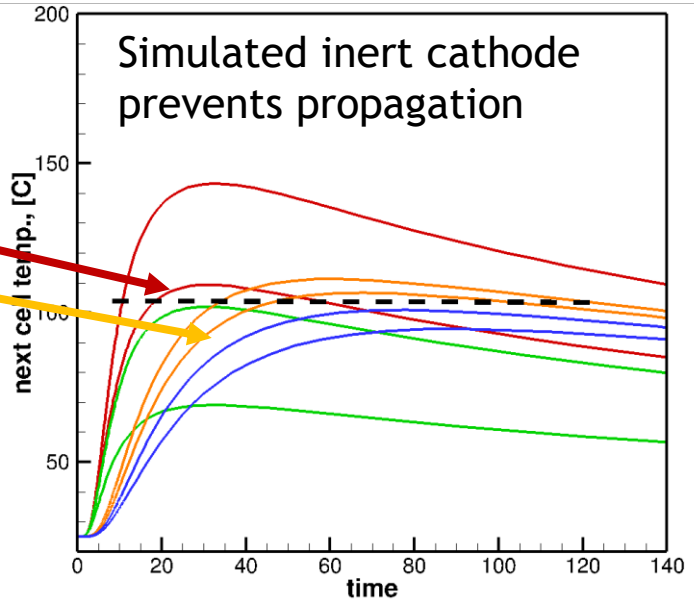

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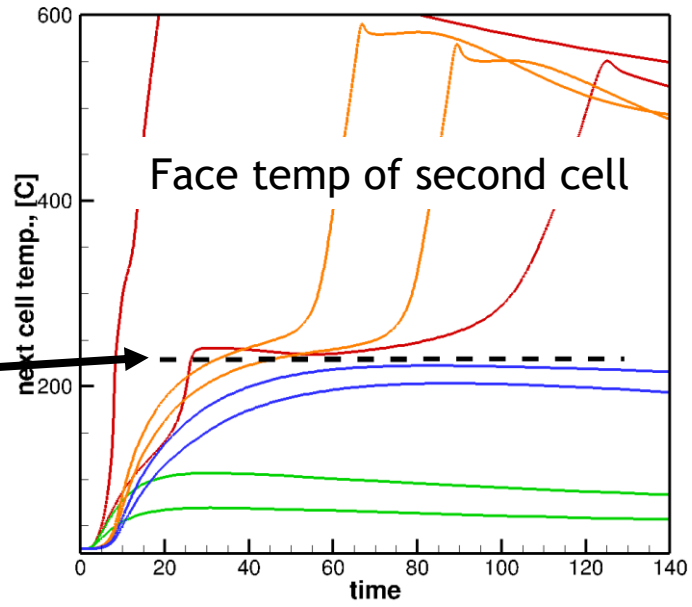

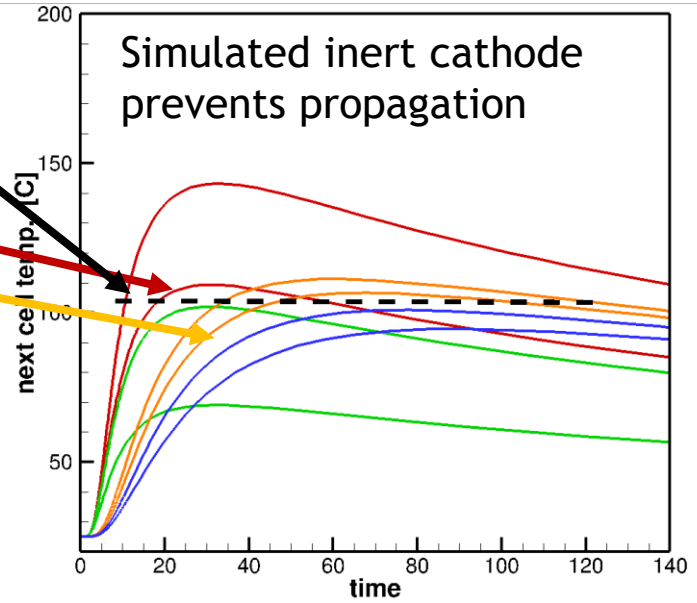

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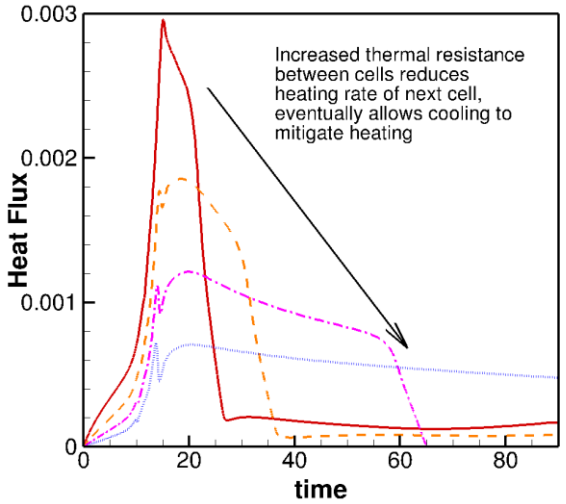
RESULTS – Opportunities with Predictive Simulations

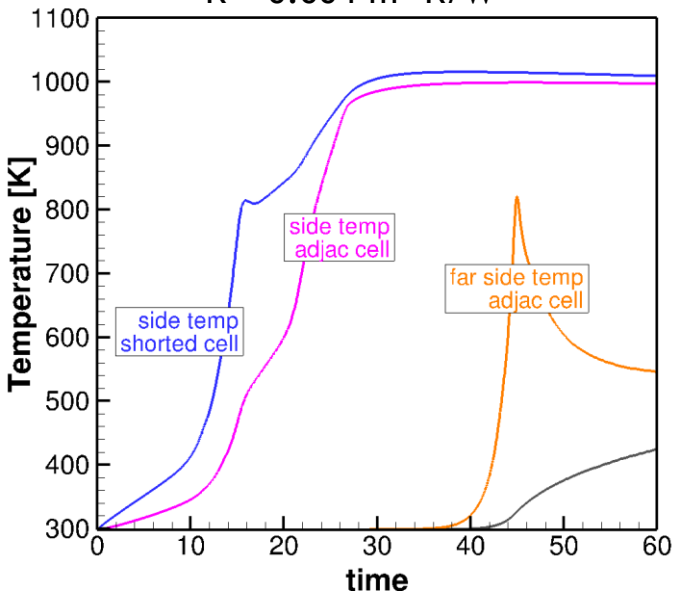
Thermal resistance between cells reduces the max heat flux between cells.

- Cell-to-cell contact resistances on the order 0.002 to 0.004 m^2*K/W.
- Thermal resistance of a few mm of insulating plastic, ceramic, etc. can increase this by 10x or more.

Heat flux between layers reduced

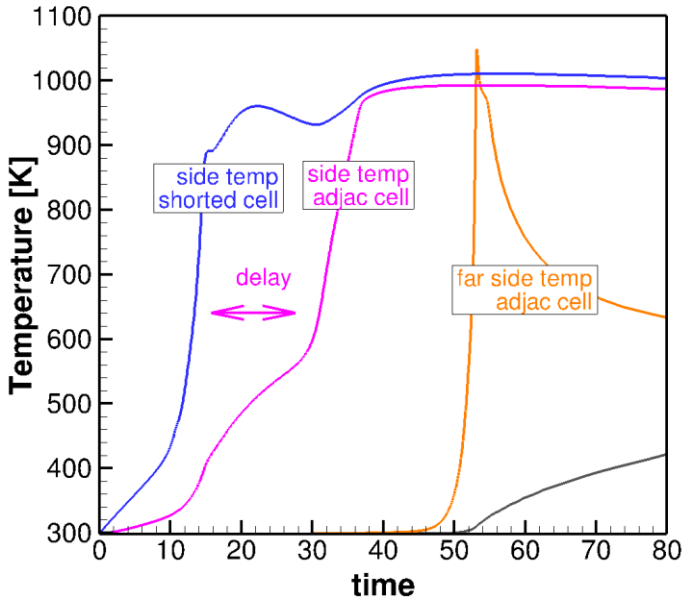


R''=0.004 m^2*K/W

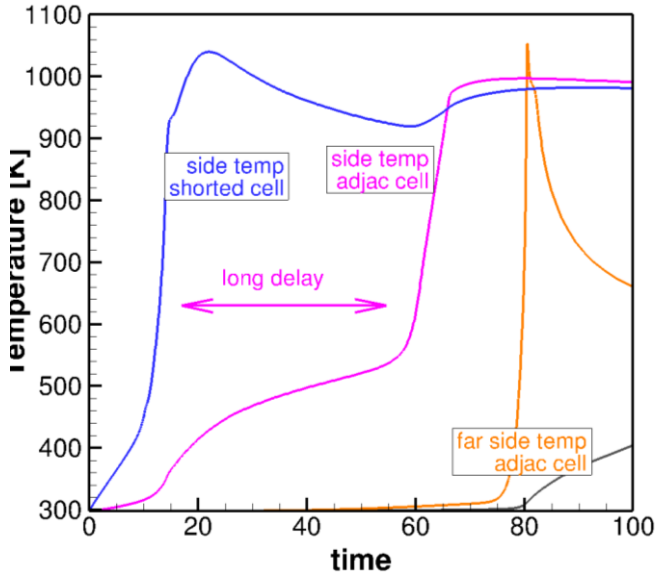


Increasing thermal resistance between layers by 2x.

R''=0.010 m^2*K/W

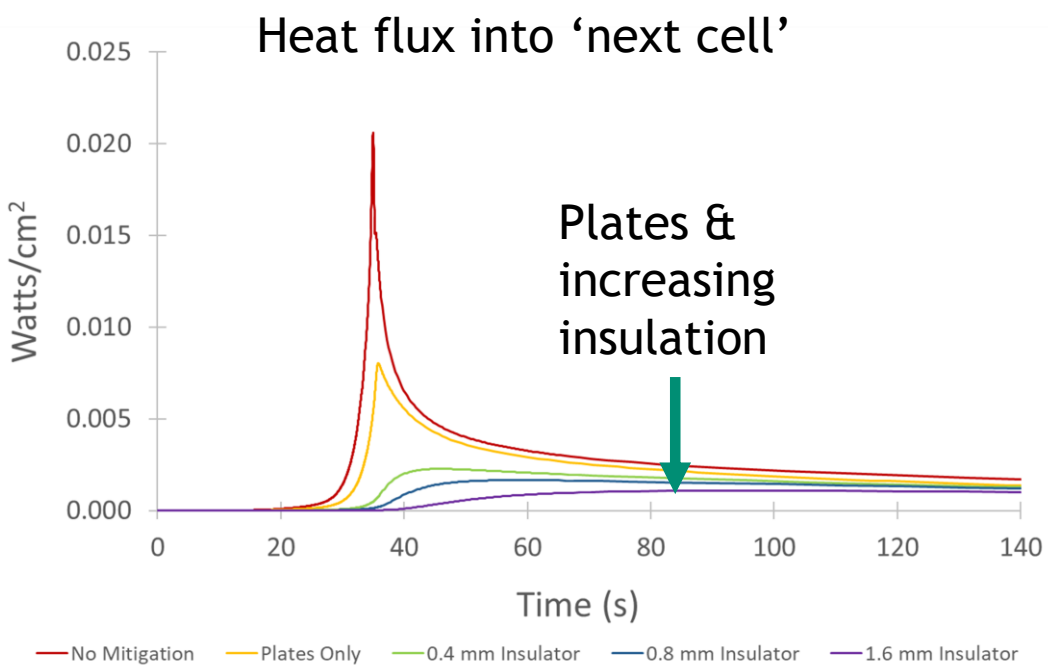


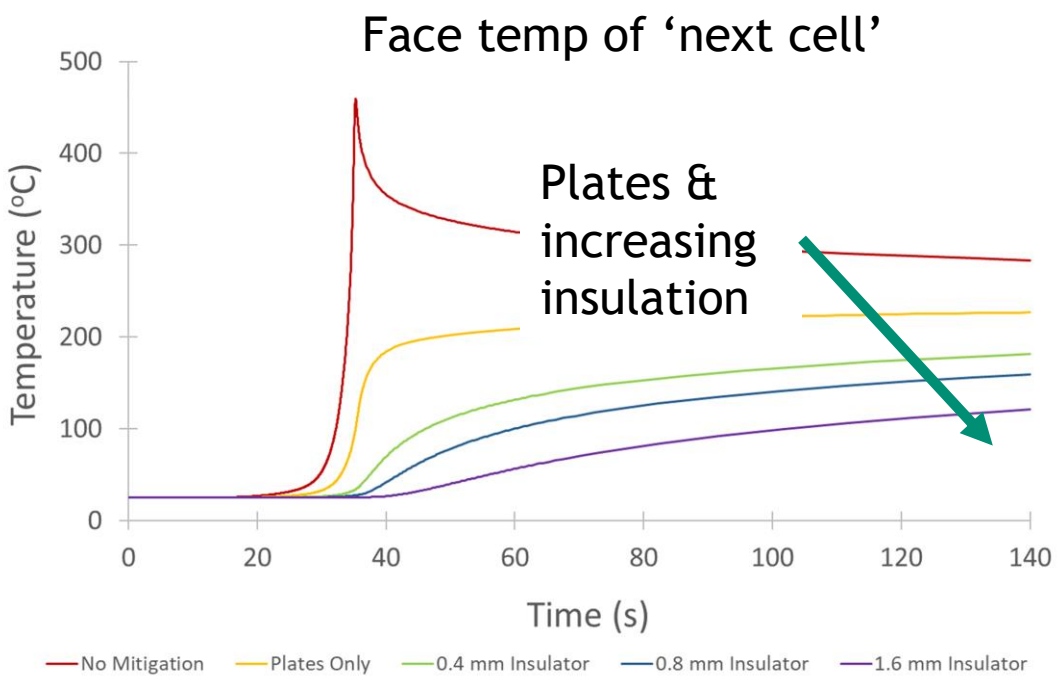
R''=0.020 m^2*K/W



Heat transfer time scales associated with active cooling project
next presentation with Loraine Torres-Castro

Insulation and structural materials delay heat transfer to adjacent cells/modules and allow for heat dissipation

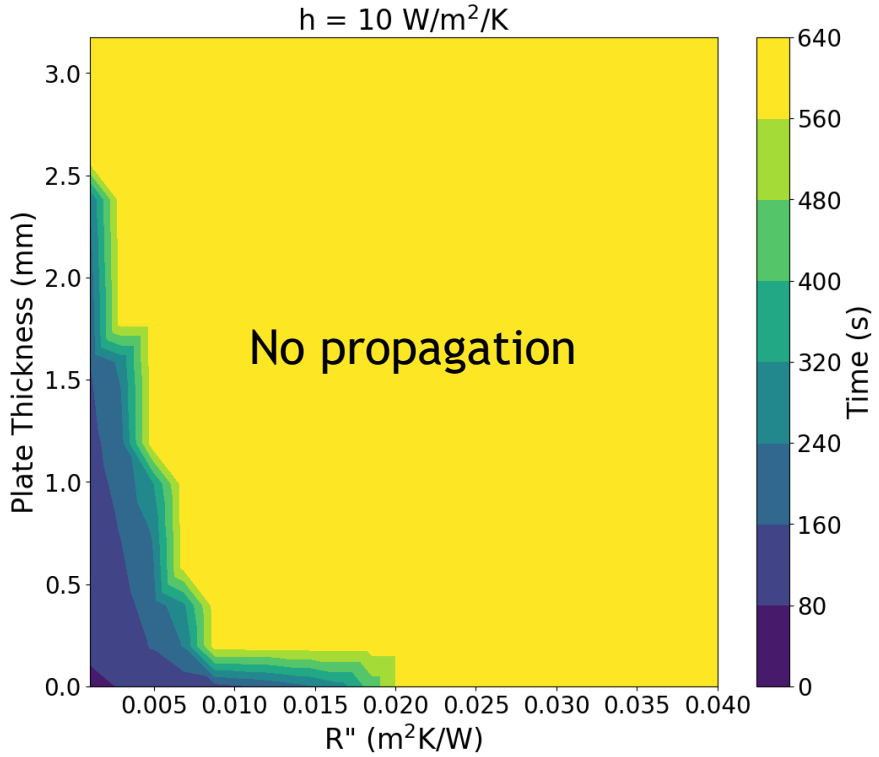




RESULTS - Predicting and Mitigating Thermal Runaway

Limits of cascading thermal runaway

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



Result here is for 3 Ah LCO cells.

Other results can be obtained through model parameter sweeps.

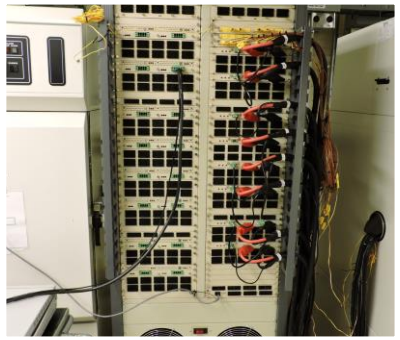
Developing LIM1TR: open source code (**L**ithium-**I**on **M**odeling for **1**-D **T**hermal **R**unaway)

Provides design tool for system design community.

Look forward to our forthcoming manuscript with analytic expressions for system design criteria

TEAM Predicting and Mitigating Thermal Runaway

Sandia Battery Test Facilities

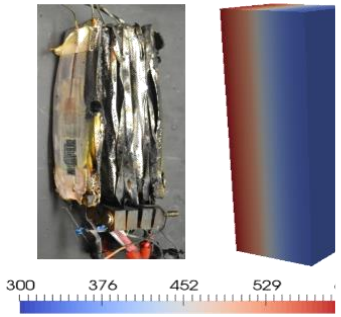


Yuliya Preger
Reed Wittman
Armando Fresquez

Sandia Battery Abuse Lab

Loraine Torres-Castro
Chris Grosso
Lucas Gray
Joshua Lamb
Jill Langendorf

Sandia Fire Sciences

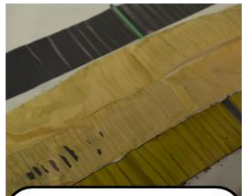


John Hewson
Randy Shurtz
Andrew Kurzawski

Center for Integrated Nanotechnologies

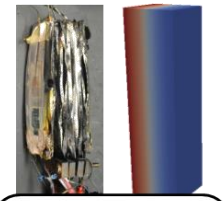
Sergei Ivanov

Baseline electrochemical performance analysis

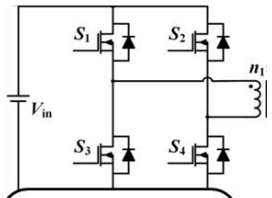


Materials characterization and thermal stability testing

Whole-cell abuse response analysis



Modeling of thermal propagation



Design of new power electronics for battery safety

PUBLICATIONS, ETC.

Peer-reviewed publications

- L. Torres-Castro, A. Kurzawski, J. Hewson, J. Lamb, "Passive mitigation of cascading propagation in multi-cell lithium ion batteries," *Journal of the Electrochemical Society*, vol. 167, 2020
- A Kurzawski, L. Torres-Castro, R. Shurtz, J. Lamb, and John Hewson, "Predicting cell-to-cell failure propagation and limits of propagation in lithium-ion stacks," *Proceedings of the Combustion Institute* (2020) https://doi.org/10.1016/j.proci.2020.06.270
- R. C. Shurtz and J. C. Hewson, "Materials Science Predictions of Thermal Runaway in Layered Metal-Oxide Cathodes: A Review of Thermodynamics," *J. Electrochem. Soc.,* 167, 090543 (2020) https://dx.doi.org/10.1149/1945-7111/ab8fd9.

Presentations

- R.C. Shurtz and J.C. Hewson "Modeling Thermal Decomposition of Metal Oxide Cathodes in Non-Aqueous Electrolytes for Prediction of Thermal Runaway in Lithium-Ion Batteries" 236th ECS Meeting, Atlanta, GA, October 17, 2019

Tools:

- A. Kurzawski, "LIM1TR: **L**ithium-**I**on **Mi**tigation for **1**-D **T**hermal **R**unaway." (approved for open source release)
- R. C. Shurtz. "Thermodynamic Reaction Heat Calculator for Layered Metal Oxide Cathodes in Organic Electrolytes" (2020) https://www.sandia.gov/ess-ssl/thermodynamic-web-calculator/

SUMMARY
Predicting and Mitigating Thermal Runaway

- Relate material models to experimental measurements at multi-cell level.

→

- Implement new high-temperature chemistry.
- Identified particle diffusion as potential high-temp physics limit.
- Provides ***comprehensive predictions of propagation and mitigation over range of conditions***.

- Address safety modeling associated with thermal modifications. Determine limits of cascading failure.

→

- Mitigate propagation with
  - increased heat capacity per stored energy.
  - thermal resistance between cells.
- Mapped out limits.
- Provide experimental design.
- ***Quantified relative effectiveness*** experimentally and through predictions.

CONTACTS

Thank you

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