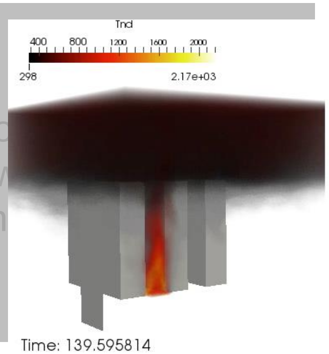


Predictive modeling for energy-storage safety in abnormal thermal scenarios

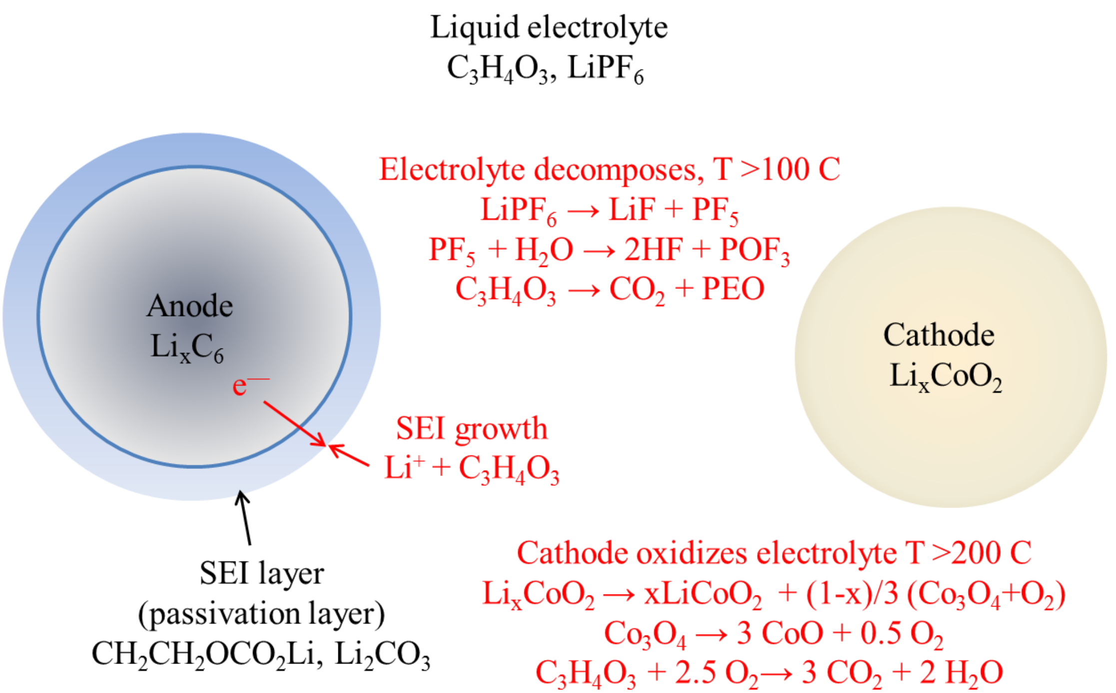
John Hewson, Randy Shurtz, Babu Chalamala, Summer Ferreira, Josh Lamb, Chris Orendorff, Erik Spoerke, Dave Ingersoll, Stefan Domino
Sandia National Laboratories

Office of Electricity Peer Review
September 27, 2016

SAND2016-9540 C

The drive to greater energy density and efficiency

- Increased energy densities and other material advances lead to more reactive systems – greater efficiency / less losses.
  - Charged batteries include a ‘fuel’ and ‘oxidizer’ all internally.
  - Li-Ion electrolyte, packaging, and other materials are often flammable.
  - External heating or internal short circuits can lead to thermal runaway.



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

- Failure rates as low as 1 in several million,
- But number of cells used in energy storage is potentially huge (billions).
- High likelihood of 'something' going wrong,
- Need to design against many possibilities.

Single Cell
~0.5-5 Ah

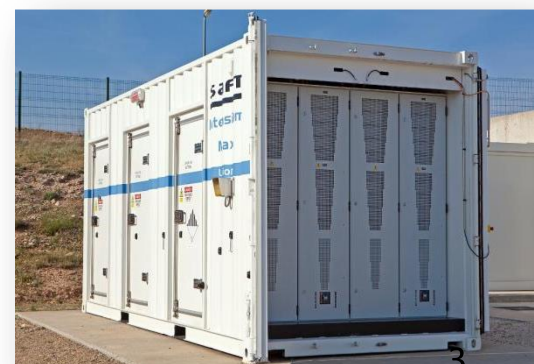
Strings and large
format cells
~10-200 Ah

EV Battery Pack 100s-
1000s cells
10-50 kWh

Stationary storage
system 1000s or more
individual cells
MWh+

- A single cell failure that propagates through the pack could lead to an impact even with very low individual failure rates

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



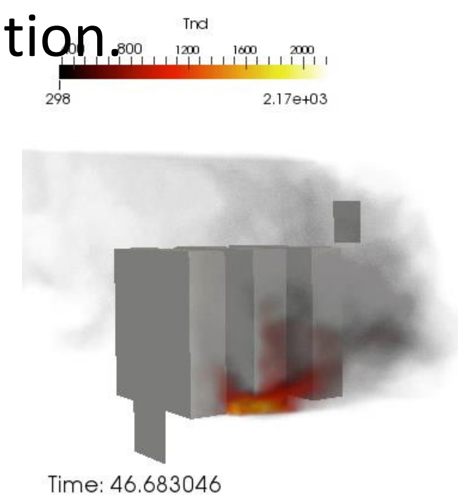
Approaches to designing in safety

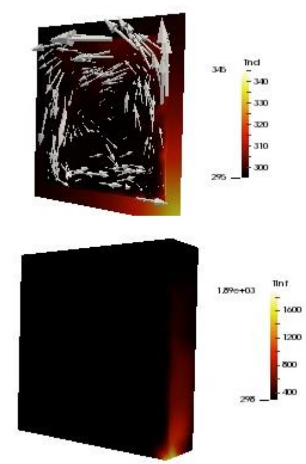
The current approach is to test our way into safety[1]

- Large system (>1MWh) testing is difficult and costly.

Consider supplementing testing with predictions of challenging scenarios and optimization of mitigation.

- Develop multi-physics models to predict failure mechanisms and identify mitigation.
- Build capabilities with small/medium scale measurements.
- Still requires some testing and validation.

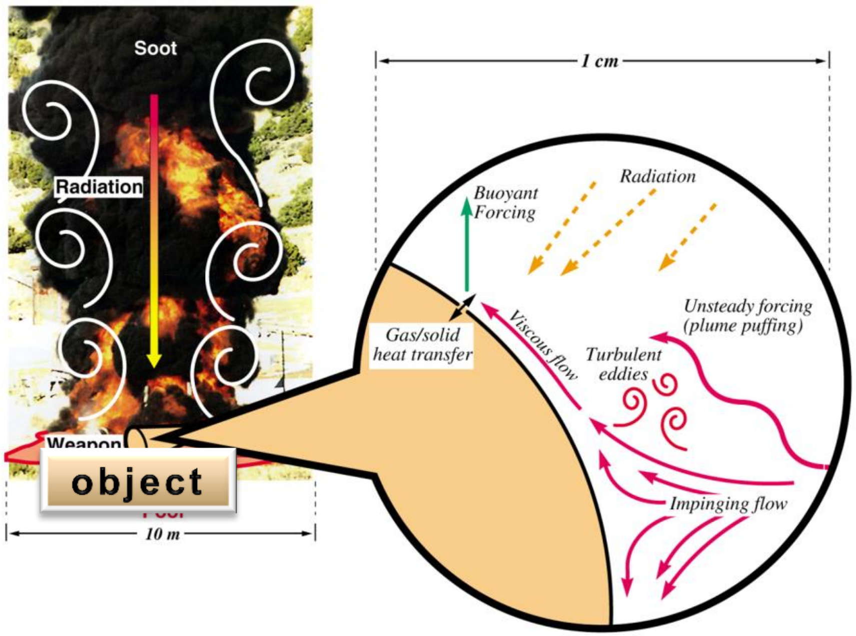




[1] 'Power Grid Energy Storage Testing Part 1.' Blume, P.; Lindenmuth, K.; Murray, J. EE – Evaluation Engineering. Nov. 2012.

How do we evaluate these terms in realistic scenarios?

- Leverage the large DOE-NNSA Investments in Sierra-Mechanics Integrated Code simulation tools developed at Sandia National Laboratories under the Advanced Scientific Computing (ASC) program for Science-based Stockpile Stewardship by applying these tools to battery safety analysis



Heat transfer mechanisms in a fire

Physics:

- Turbulent fluid mechanics (buoyant plumes)
- Participating Media Radiation (PMR)
- Reacting flow (hydrocarbon, particles, solids)
- Conjugate Heat Transfer (CHT)
- The simulation tool *predicts* the thermal environment and object response

Predicting fire environments and consequential heating

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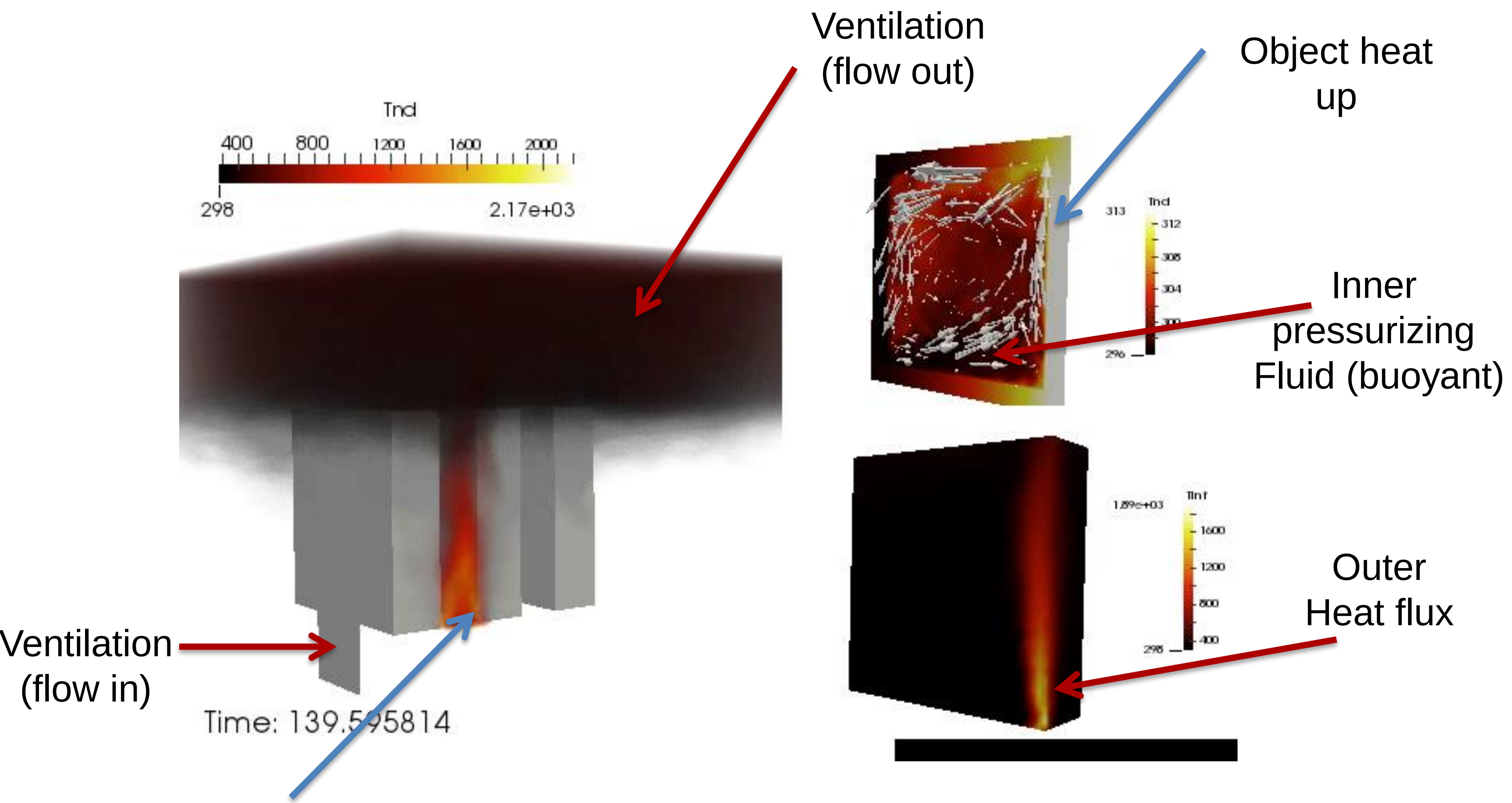

Fire modeled as a combustible hydrocarbon

Multi-physics coupling

Sandia National Laboratories

The equations and couplings…

Fluid/Thermal

Fluids:

$$\frac{\partial \bar{\rho}\tilde{h}}{\partial t}+\frac{\partial}{\partial x_j}\bar{\rho}\,\tilde{h}\tilde{u}_j=-\frac{\partial}{\partial x_j}\left(\bar{q}_j+\tau_{hu_j}\right)-\frac{\partial \bar{q}_i^r}{\partial x_i}+\frac{\partial P}{\partial t}+\tilde{u}_j\frac{\partial P}{\partial x_j}+\tau_{ij}\frac{\partial u_i}{\partial x_j}$$

Thermal:

$$\rho C_P\frac{\partial T}{\partial t}+\frac{\partial}{\partial x_j}q_j=S_T$$

Coupling:

$$q_j^s n_j^s=q_j^f n_j^f$$

PMR/Thermal

RTE:

$$s_j\frac{\partial}{\partial x_j}I(\vec{r},s)+(\bar{\mu}_a+\bar{\mu}_s)I(\vec{r},s)=\overline{\mu_a I_b}+\mu_s\frac{G}{4\pi}$$

Thermal:

$$\rho C_P\frac{\partial T}{\partial t}+\frac{\partial}{\partial x_j}q_j=S_T$$

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Fluid/PMR

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RTE:

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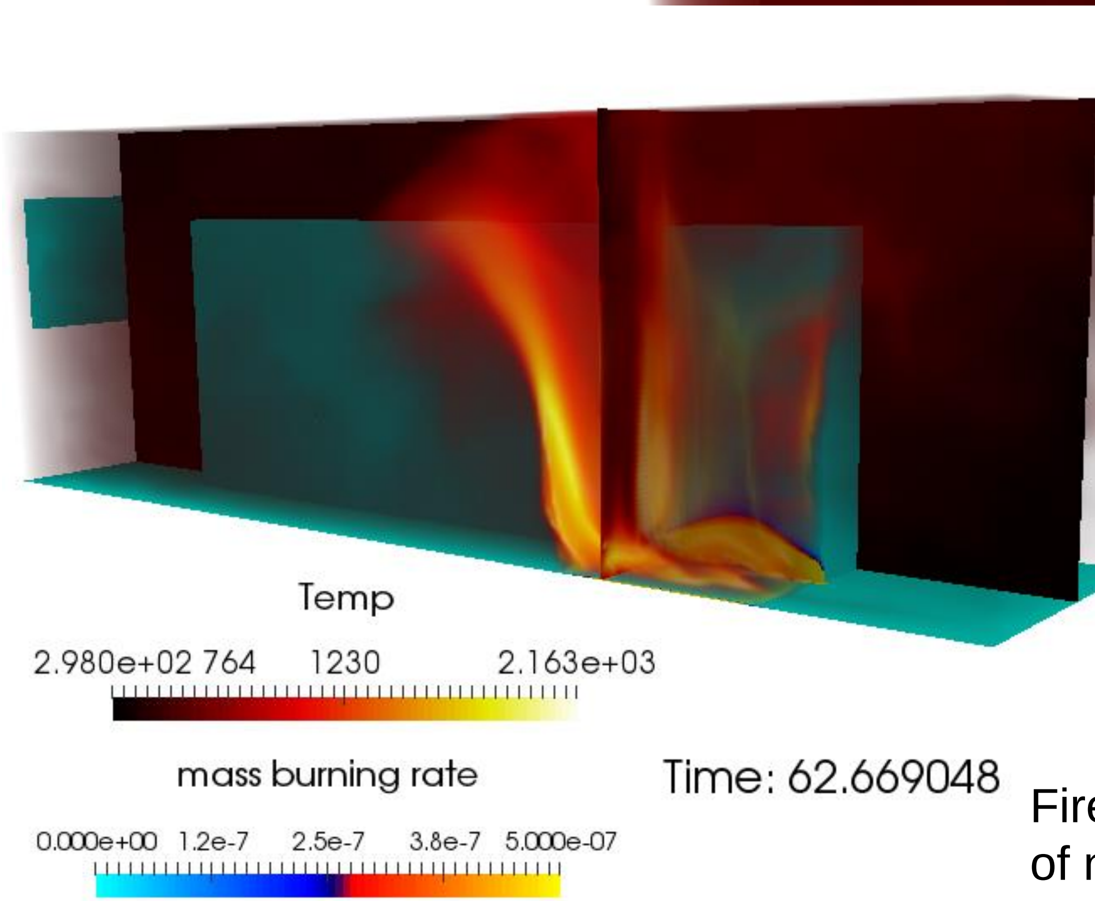
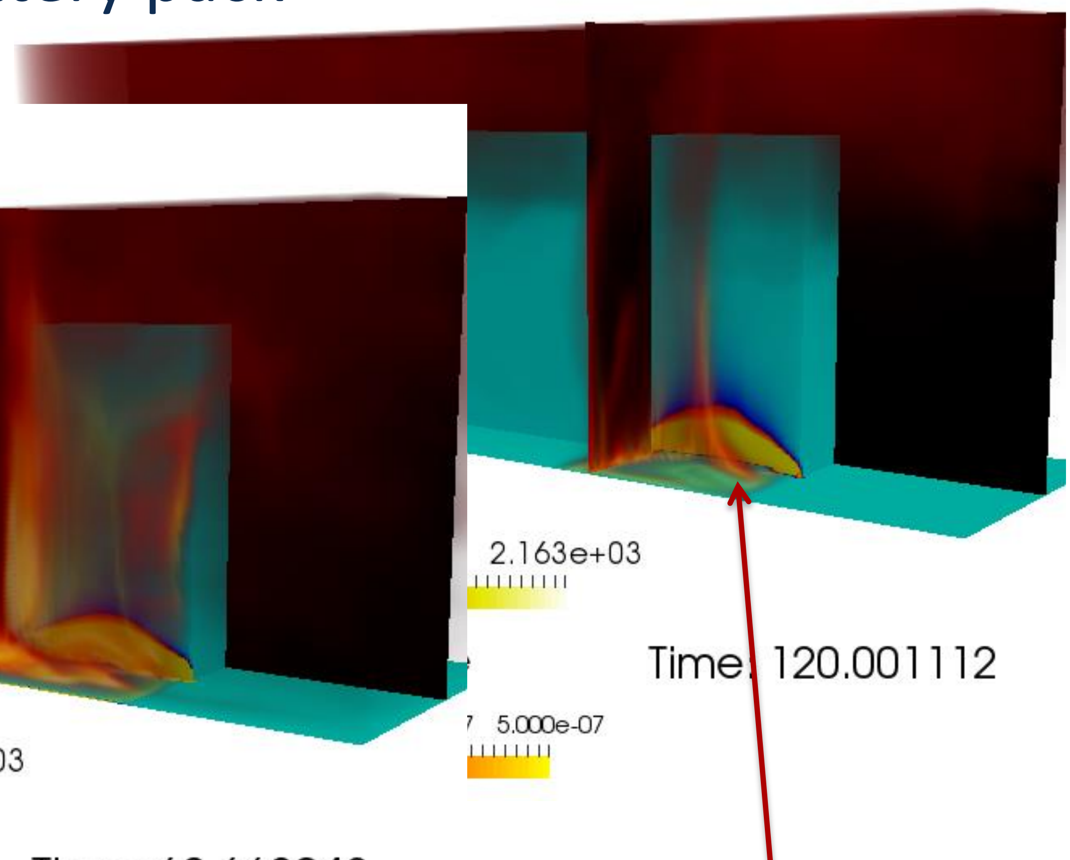
Coupling:

$$\frac{\partial \bar{q}_i^r}{\partial x_i}=\mu_a\left[4I_b-G(\vec{r})\right]$$

From predicting fire environments to predicting heat release in a battery pack



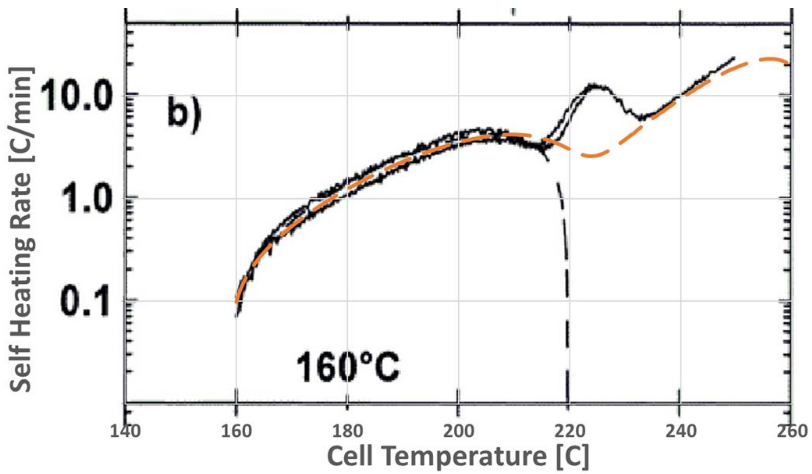


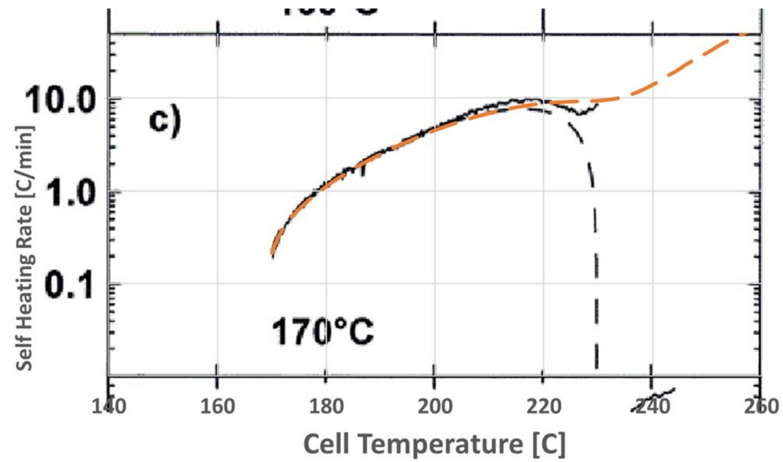
Fire environment results in heating of notional battery pack.

Now focus on what happens to that heated battery pack.

Development of heat release models from calorimetry measurements

- Calorimetry measurements inform and calibrate models for heat release rates.
- Here cathode heat release models are evaluated based on literature measurements.
- These heat release models are in our codes and used in subsequent predictions.



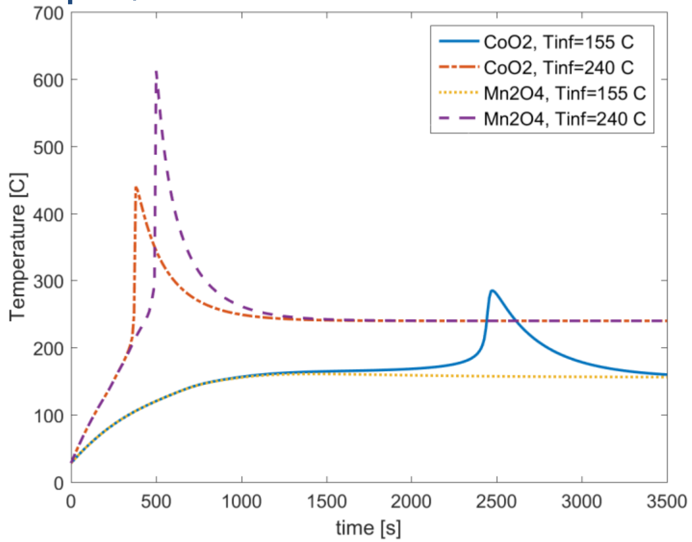


- Measurement from: MacNeil, D. D. and J. R. Dahn (2001). "Test of reaction kinetics using both differential scanning and accelerating rate calorimetries as applied to the reaction of LixCoO2 in non-aqueous electrolyte."
- Models based on Spotnitz, R. and J. Franklin (2003). "Abuse behavior of high-power, lithium-ion cells." Journal of Power Sources **113**(1): 81-100.

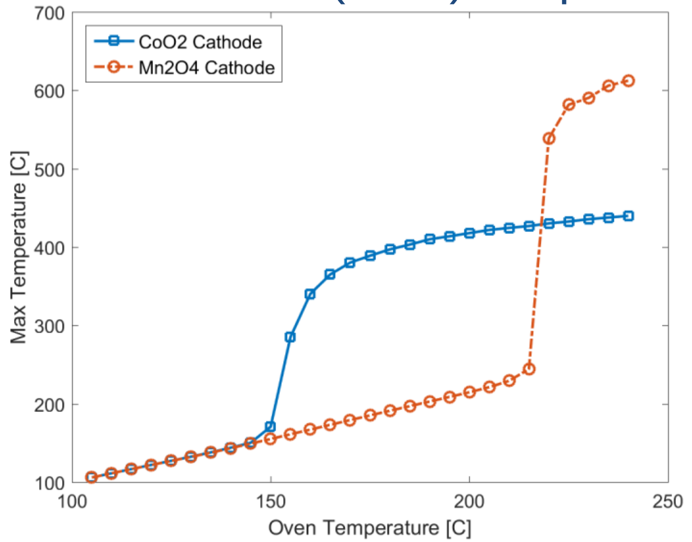
Modeling thermal runaway in lithium ion cells

- Evolution simulated using calorimetry-derived heating rates and lumped thermal mass.
- Consider SEI decomposition, cathode-electrolyte reaction, electrolyte decomposition, anode-electrolyte reaction
- Fire environment modeled as an ambient temperature.
- Bound thermal runaway versus heat dissipation.

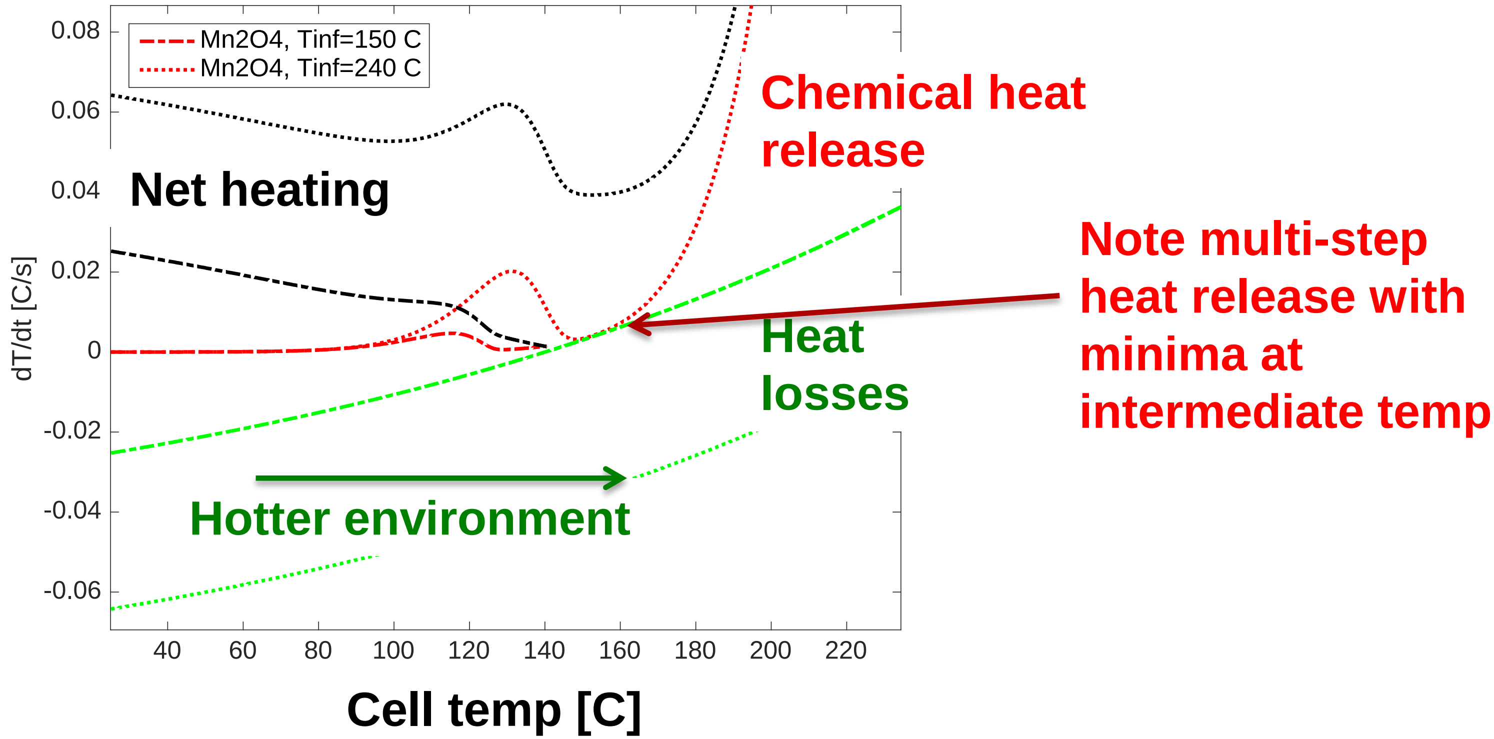
Temp. evolution two environ. temps., two cathode materials



Max temp. predicted versus environment (oven) temp.

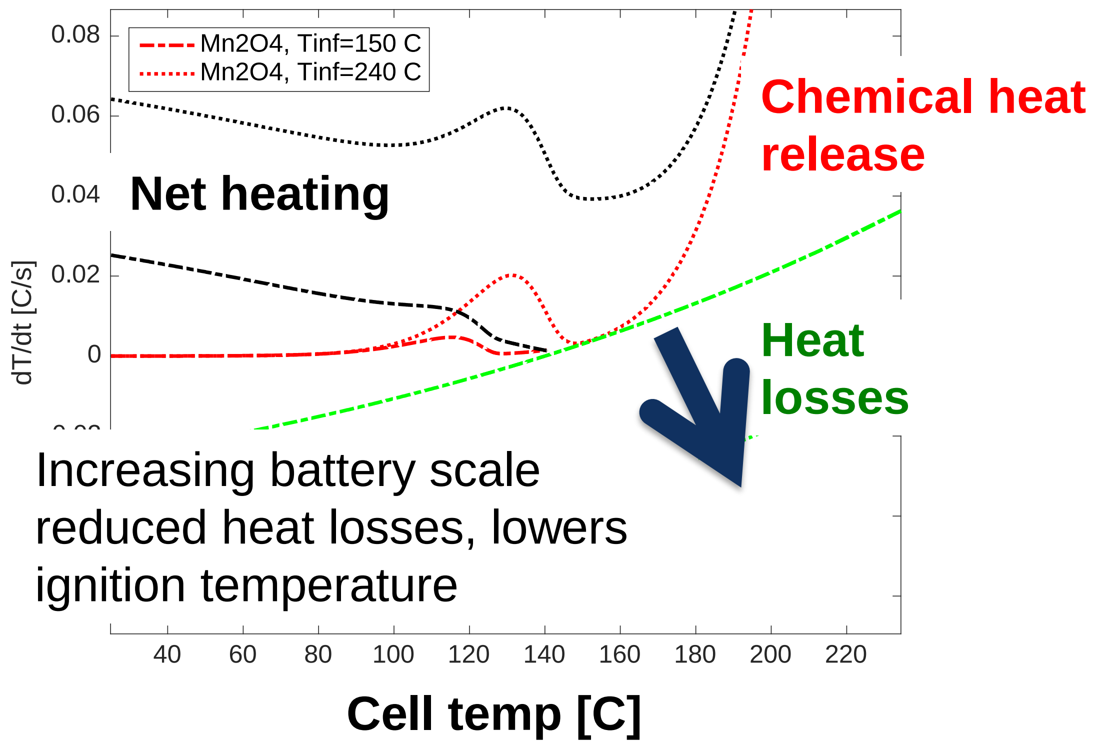


Thermal runaway occurs if heat release exceeds heat losses



- Predicted heating rates based on ARC measurements.
- Higher environment temperature leads to thermal runaway.
- Low temperature degradation occurs in both cases.

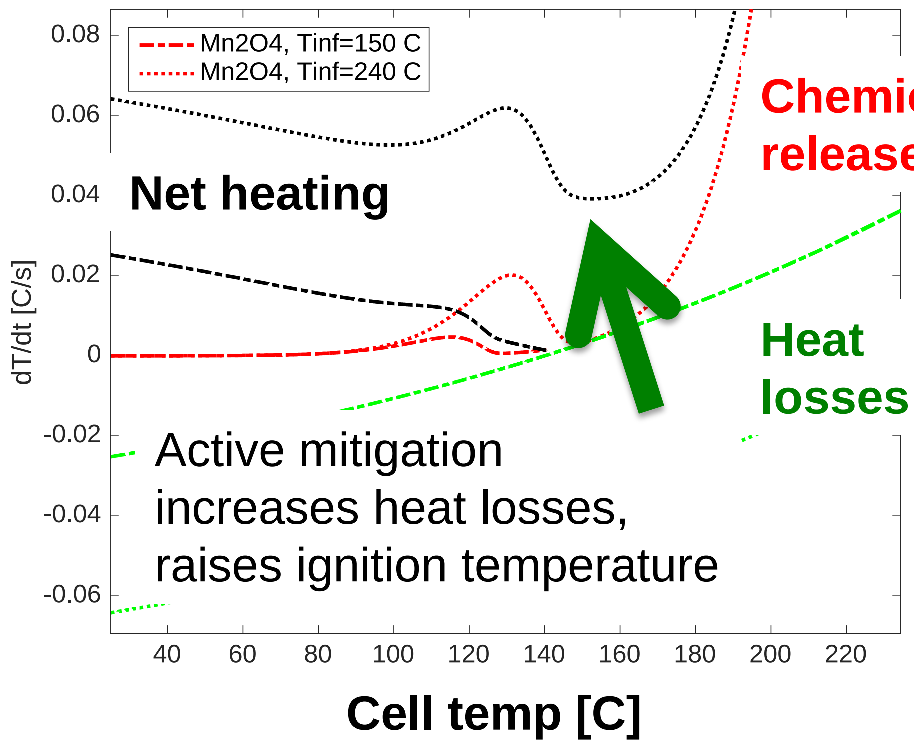
Thermal runaway occurs if heat release exceeds heat losses



- Criterion for self heating:

$$\Delta H[C]^n A e^{-E/RT} + \dot{q}_{internal} > h_{eff}\left(S/V\right)\left(T - T_{\infty}\right)$$

Thermal runaway occurs if heat release exceeds heat losses



But, if the temperature dependence is strong, sensitivity to scale and heat losses is small.

Focus mitigation on shallow-sloped regions!

- Criterion for self heating:

$$\Delta H[C]^n A e^{-E/RT} + \dot{q}_{internal} > h_{eff}\left(S/V\right)\left(T - T_\infty\right)$$

Failure of a single cell can propagate to rest of pack

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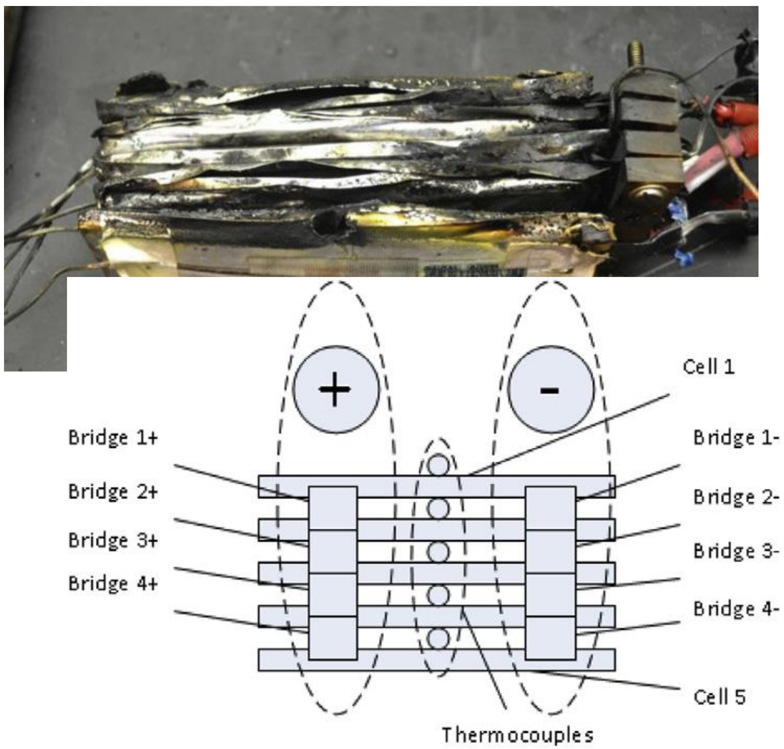
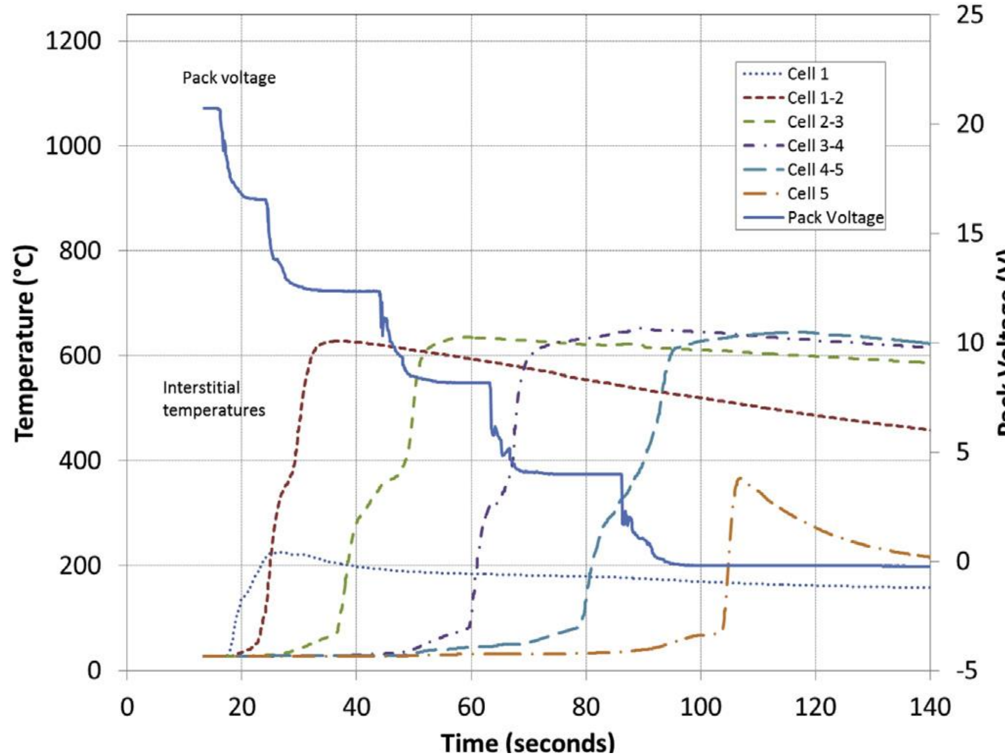
Experimental propagation in 5 stacked pouch cells

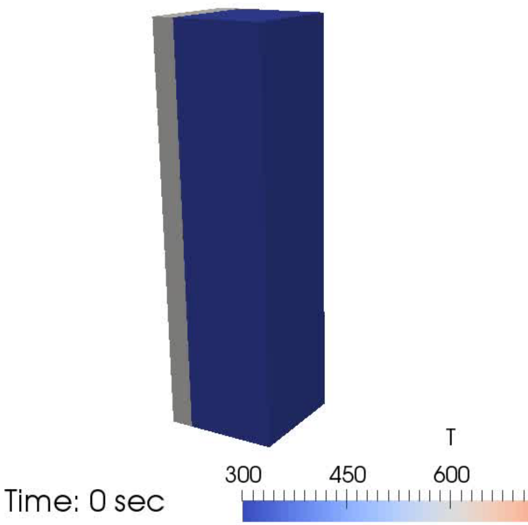


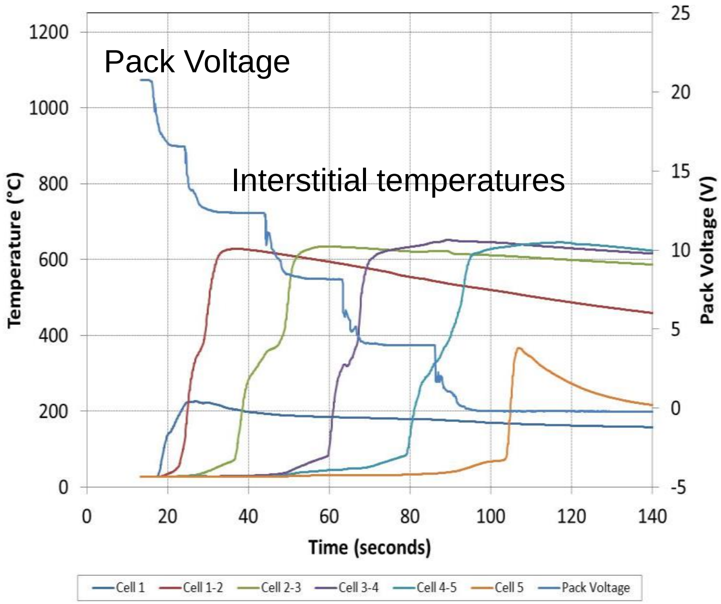


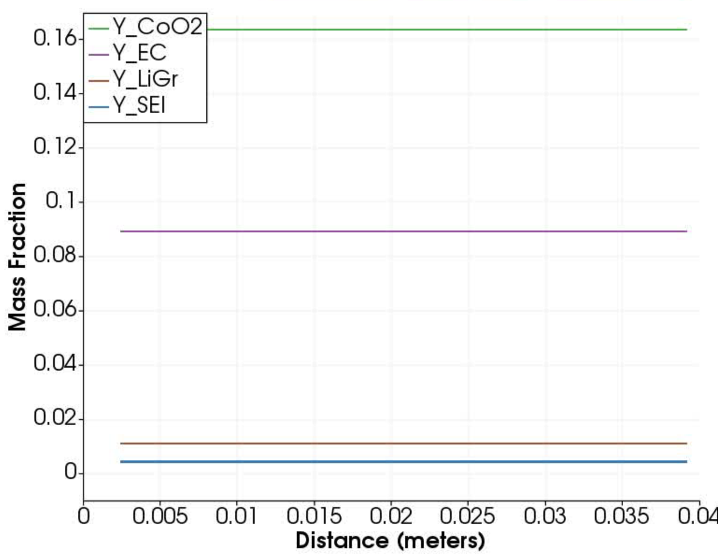
Lamb, J., et al. (2015). Journal of Power Sources **283**: 517-523.

Propagation across multiple (5) cells

- Prediction and mitigation of cell-to-cell propagation is key to addressing risk.
- Here simulating propagation across series of pouch cells.
- Accurate measurements of highest temperature kinetics unavailable and need to be calibrated to get agreement.







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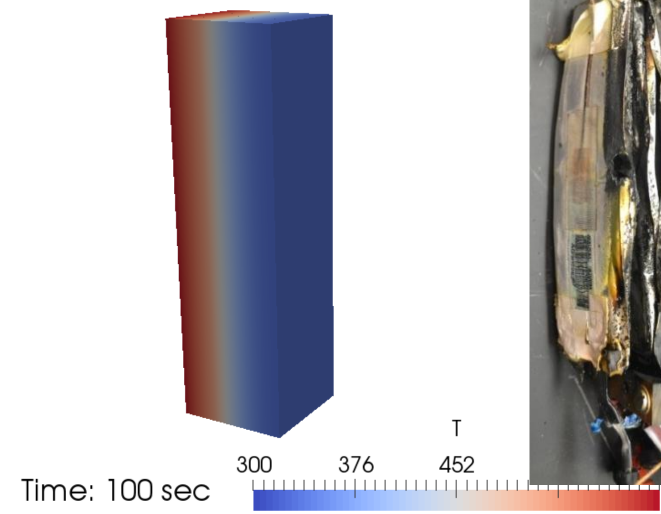
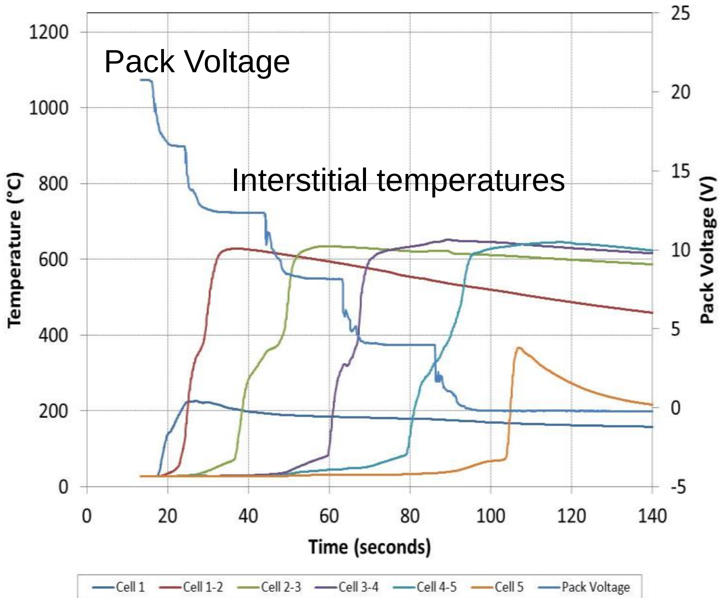
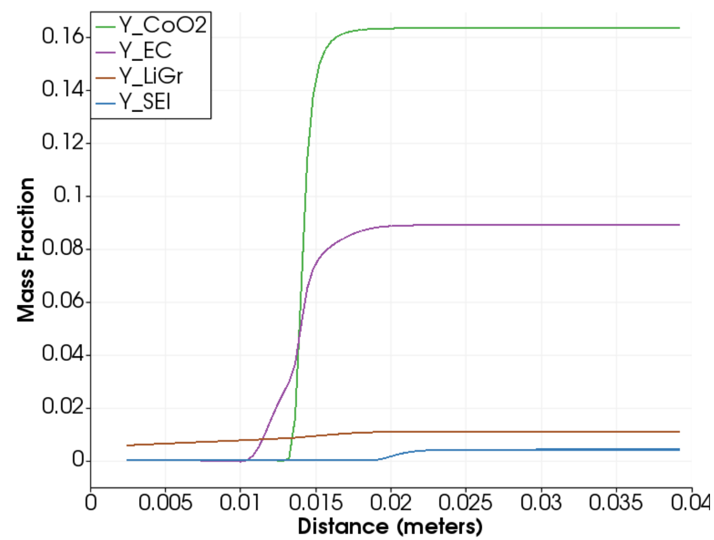
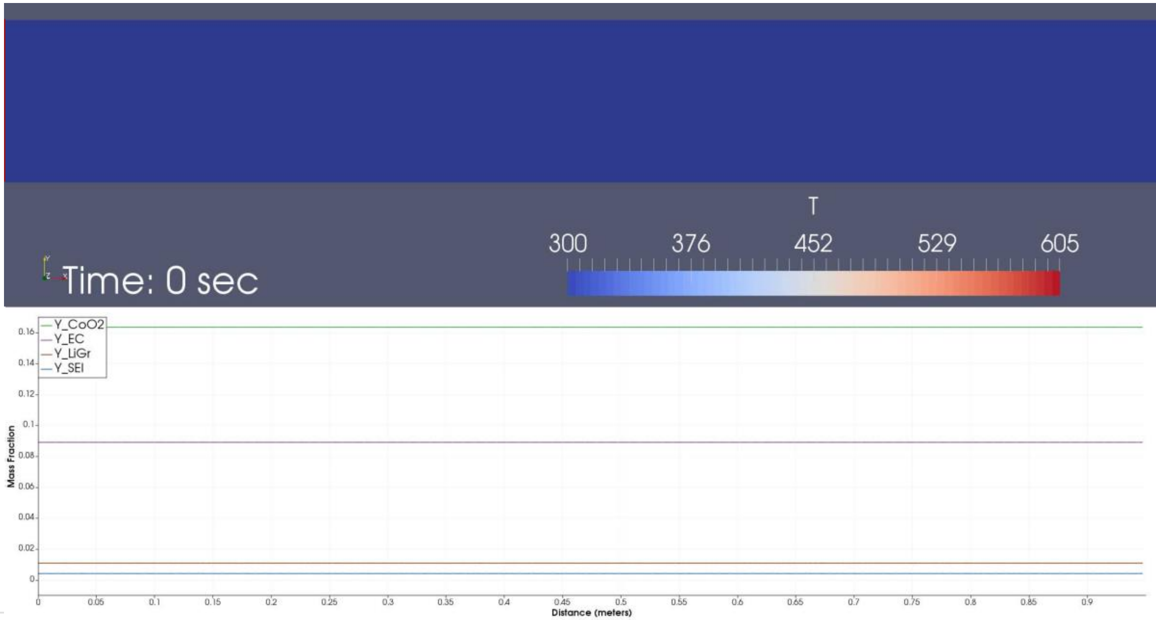


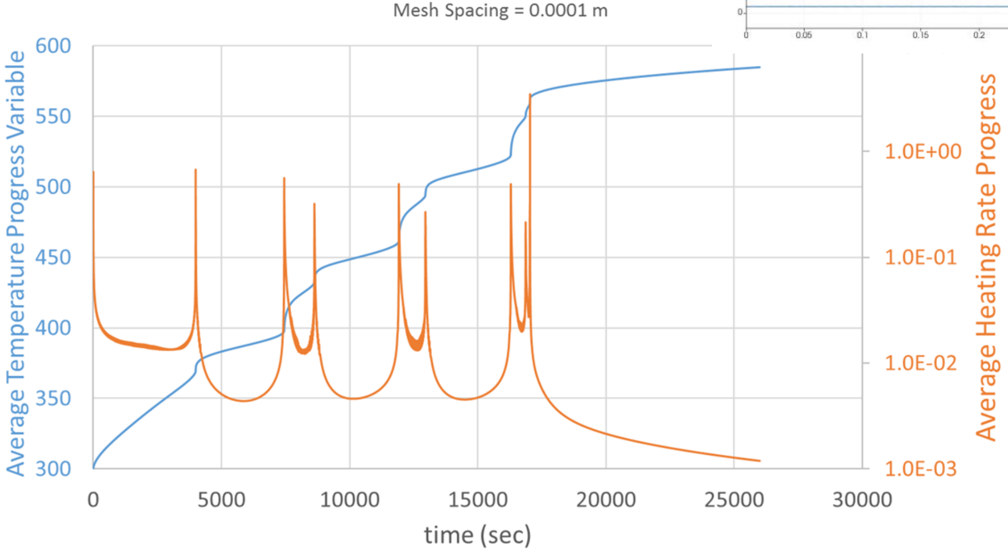




Pulsating Propagation at large scales

- Extend modeling to large scales at small cost relative to measurements.
- Prediction and mitigation of cell-to-cell propagation is key to addressing risk.
- Here predictions include multi-step mechanism involving anode, cathode, electrolyte reactants.





- Propagation across a large pack (128 cells here) exhibits pulsating instabilities.
- Note heating rate varies by 100x (log scale).

Pulsating Propagation at large scales

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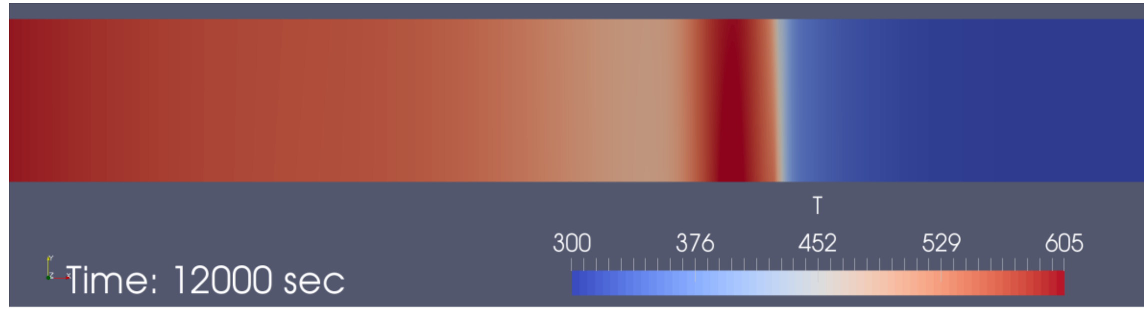
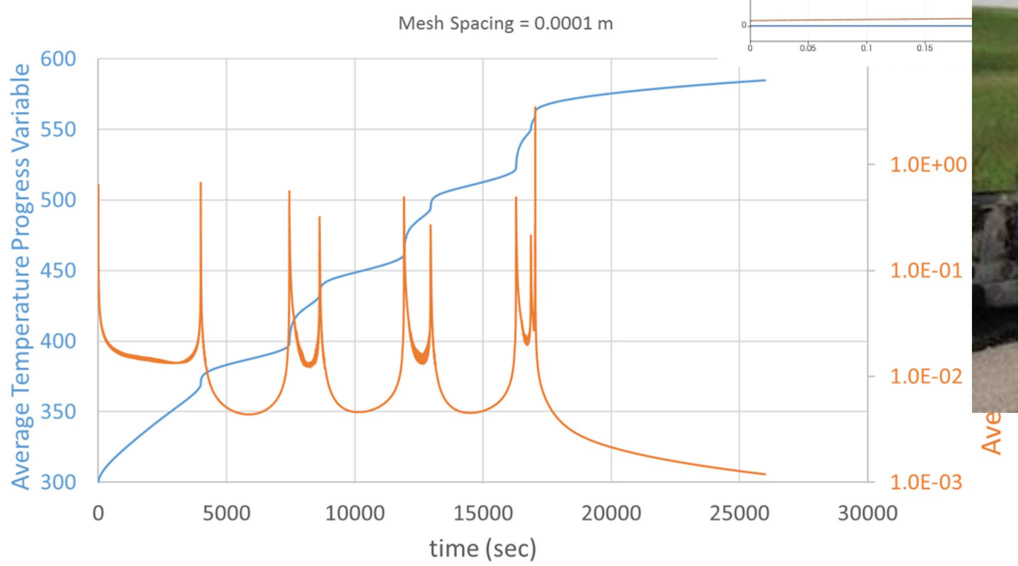


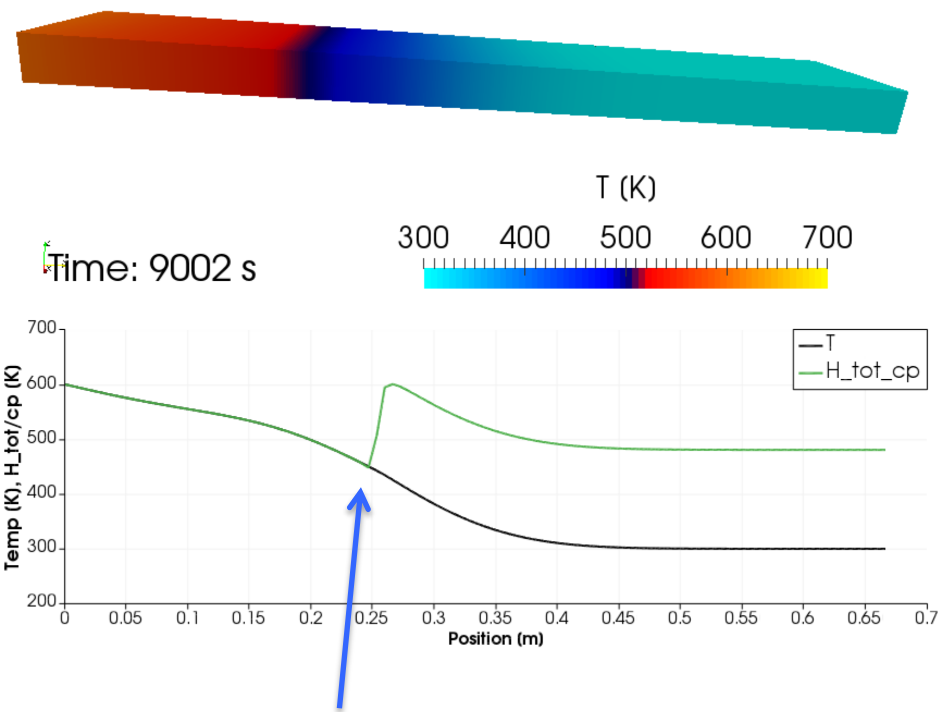
2011 Chevy Volt Latent Battery Fire at DOT/NHTSA Test Facility

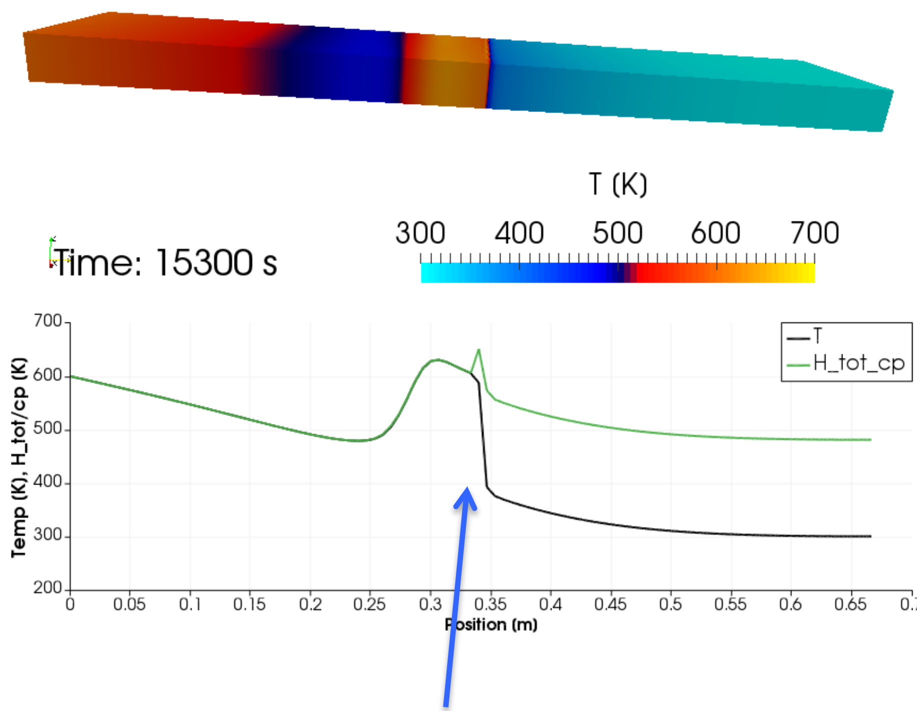


- Note heating rate varies by 100x (log scale).

The mechanism of pulsating propagation

- Heat released is conducted upstream of reaction front, increasing the total enthalpy (sum of sensible and chemical enthalpy) $H_{TOT} = c_p T + Y_r \Delta H_r$
- Front propagates rapidly through preheated region with larger H_{TOT}.





- Slow propagation (low Temp), but preheating mixture ahead of reaction front.
- Rapid propagation (high Temp), into preheated mixture.

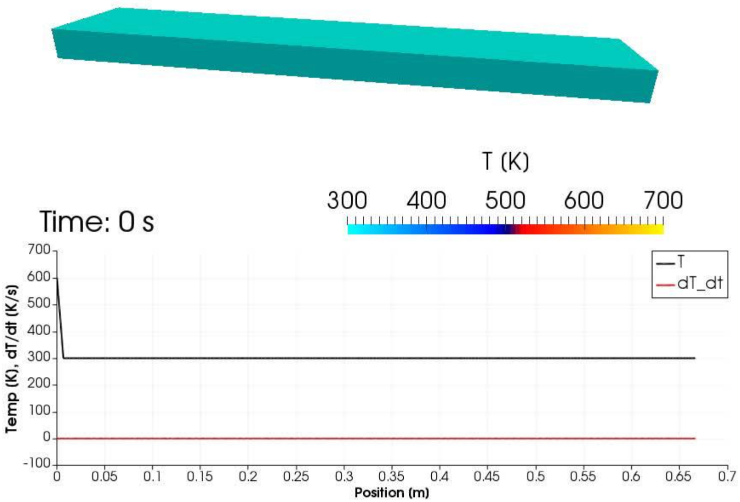
Parameter studies of propagation at large scales are possible with models

- Prediction and mitigation of cell-to-cell propagation is key to addressing risk.
- Single-step heat-release predictions with a range of heat release and boundary temps.
- Propagation across a large pack (80 cells here) exhibits pulsating instabilities.

$$\frac{Y_r \Delta H_r}{c_p} = 184\ \mathrm{K} \qquad T_{left} = 450\ \mathrm{K}$$

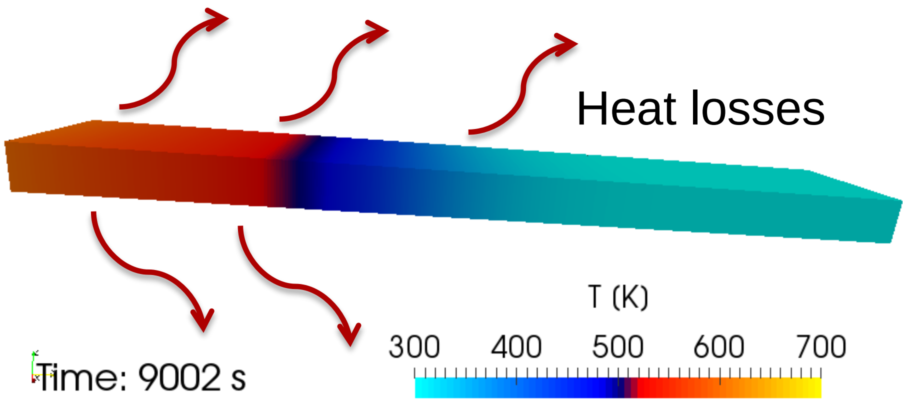
$$\frac{Y_r \Delta H_r}{c_p} = 276\ \mathrm{K} \qquad T_{left} = 450\ \mathrm{K}$$

$$\frac{Y_r \Delta H_r}{c_p} = 184\ \mathrm{K} \qquad T_{left} = 600\ \mathrm{K}$$



Future work

- Fit historical data from a variety of battery chemistries (Sandia BattLab and literature) to kinetic models.
- Identify cell-pack configurations that inhibit initial ignition.
- Model thermal interaction of battery packs in Sierra.
  - Predict configurations leading to cascading versus isolated failure.
  - Focus on heat losses required to mitigate propagation.



- Intermediate term
  - Integrate reacting thermal model of battery packs with fire models in Sierra to evaluate safety of representative geometries and scenarios.
  - Predict contributions of battery thermal runaway to overall fire load and as source of hazardous products.
- → **Ultimate goal:** ***Predict criteria for cascading failure to act as a design tool in developing mitigation strategies.***

Publications and presentations

- Publications
  - Ferreira, S.R., et al., *Fundamental aspects of the safety of large-scale energy storage systems, Paper 5.3*, in *Power Sources Conference*. 2016: Orlando, FL.
  - Hewson, J.C., *Understanding the limits of thermal runaway in lithium-ion battery systems*, in *Interflam*. 2016: London, UK.

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  - Hewson, J.C., *Understanding the limits of thermal runaway in lithium-ion battery systems*, in *Interflam*. 2016: London, UK.

In closing

- Thermal runaway is a significant risk and potential barrier to development and acceptance.
- Simple thermal models coupled with knowledge of fire environment can potentially identify critical ignition and propagation trends.
- Quality measurements are key to parameter identification.
- Progress this term in
  - Development of thermal source terms.
  - Integration of source terms in ASC multi-physics code framework.
  - Identification of thermal ignition criterion.
  - Cell-to-cell propagation along homogenized pack structures.

Acknowledgements

- Supported by Imre Gyuk and the OE Electrical Energy Storage Program.
  - Early work was supported by the Sodium-based batteries task under the leadership of David Ingersoll and Eric Spoerke.

- Collaborative discussions with Summer Ferreira, Josh Lamb, Chris Orendorff, Dave Ingersoll and Stefan Domino have been instrumental in