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THERMAL RUNAWAY AT SCALE: ANALYZING ESS SAFETY WITH MODULE TO RACK SCALE MODELS

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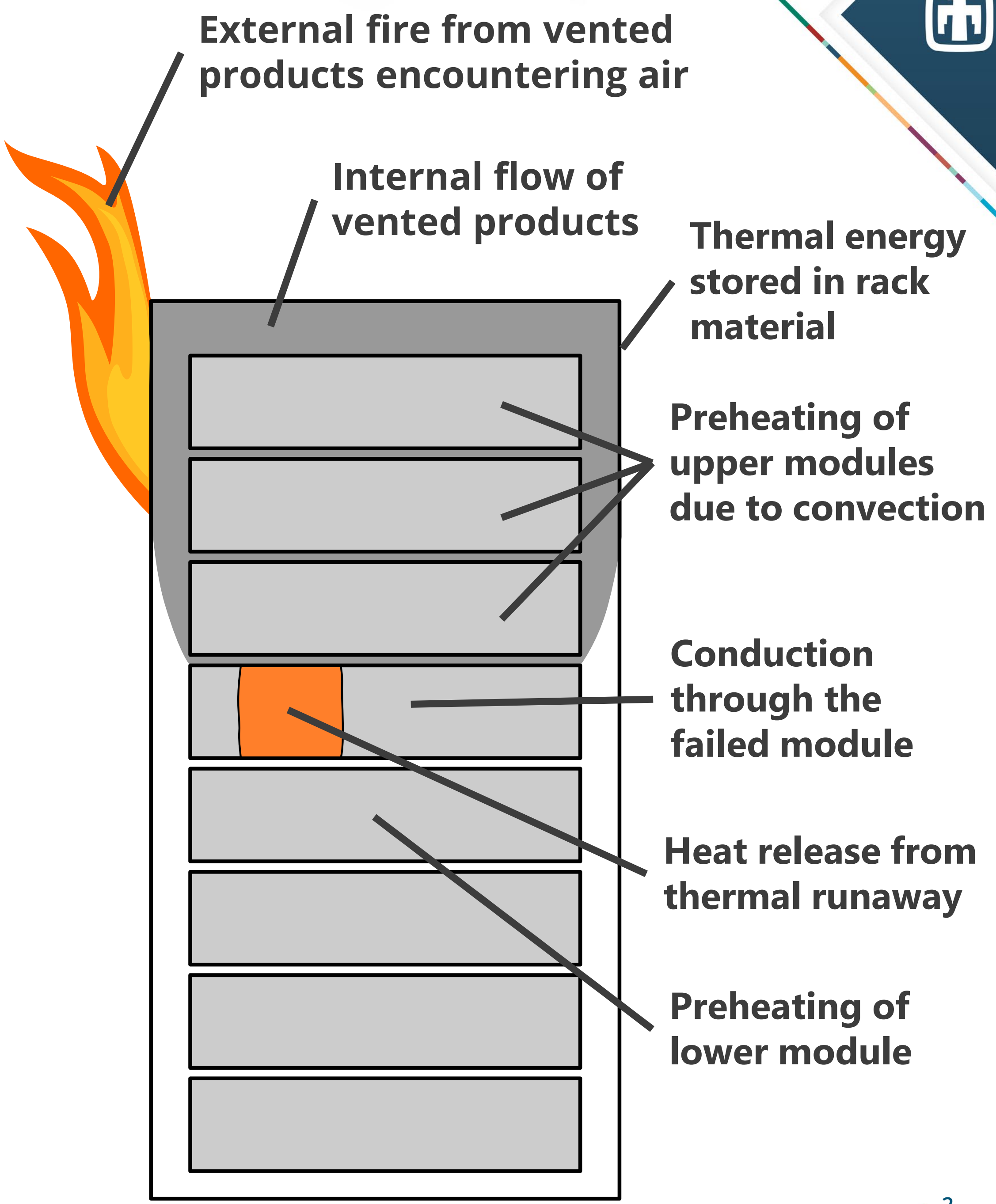
THERMAL RUNAWAY MODELING

- Rich history of cell-level thermal runaway modeling dating back over 20 years
- Applying these models at larger (module/rack) scales presents additional challenges
- Scale of problem can be defined by heat transfer:
  - Fast: internal cell heating
  - Medium: cell-to-cell heat transfer
  - Slow: module-to-module interactions
- How can models improve our understanding of system-level safety?



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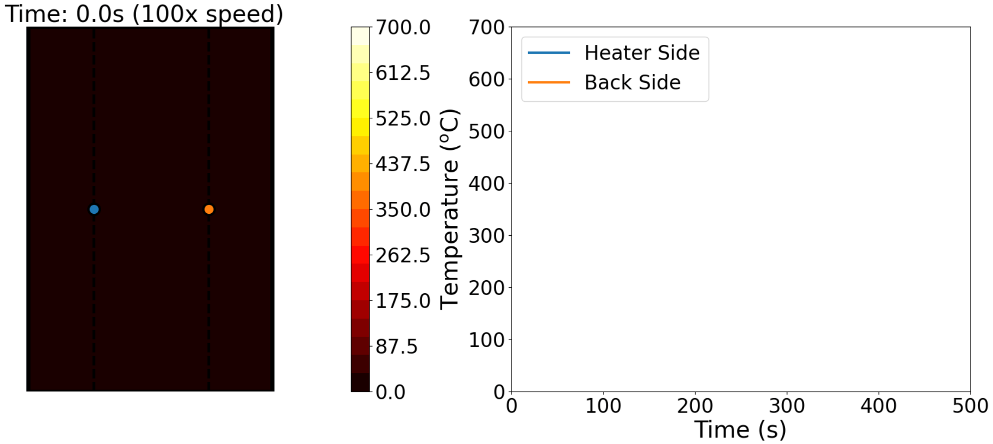
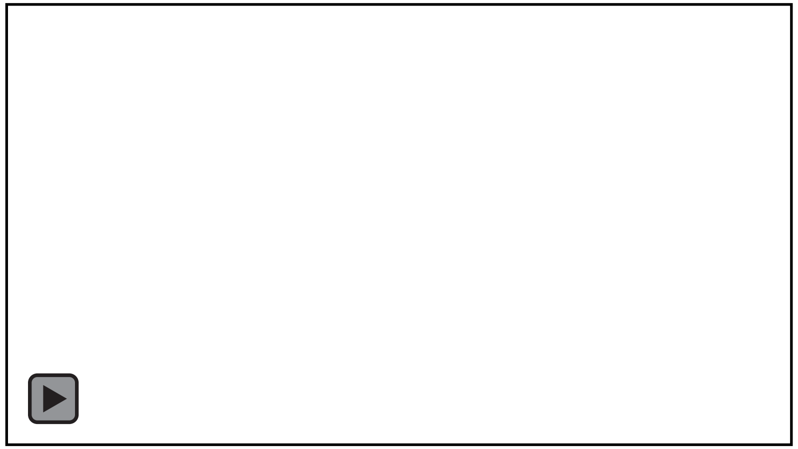
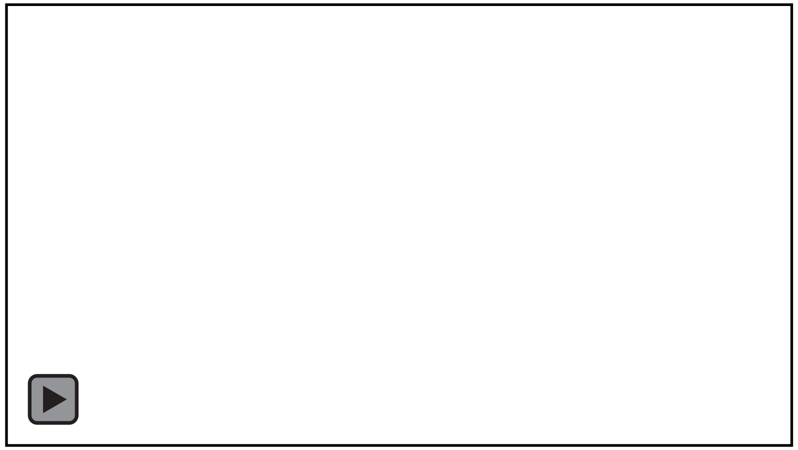
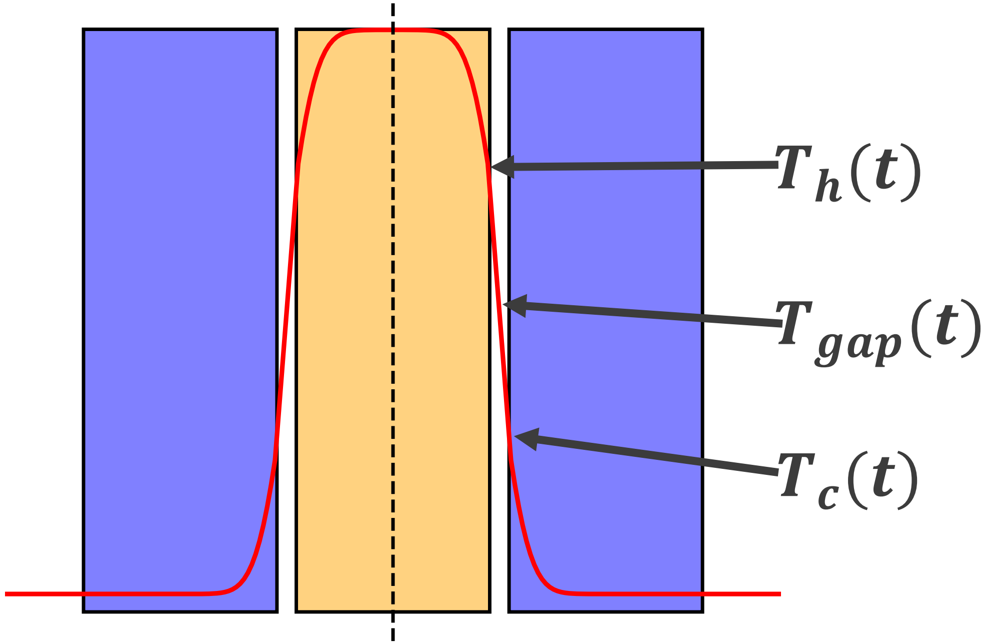


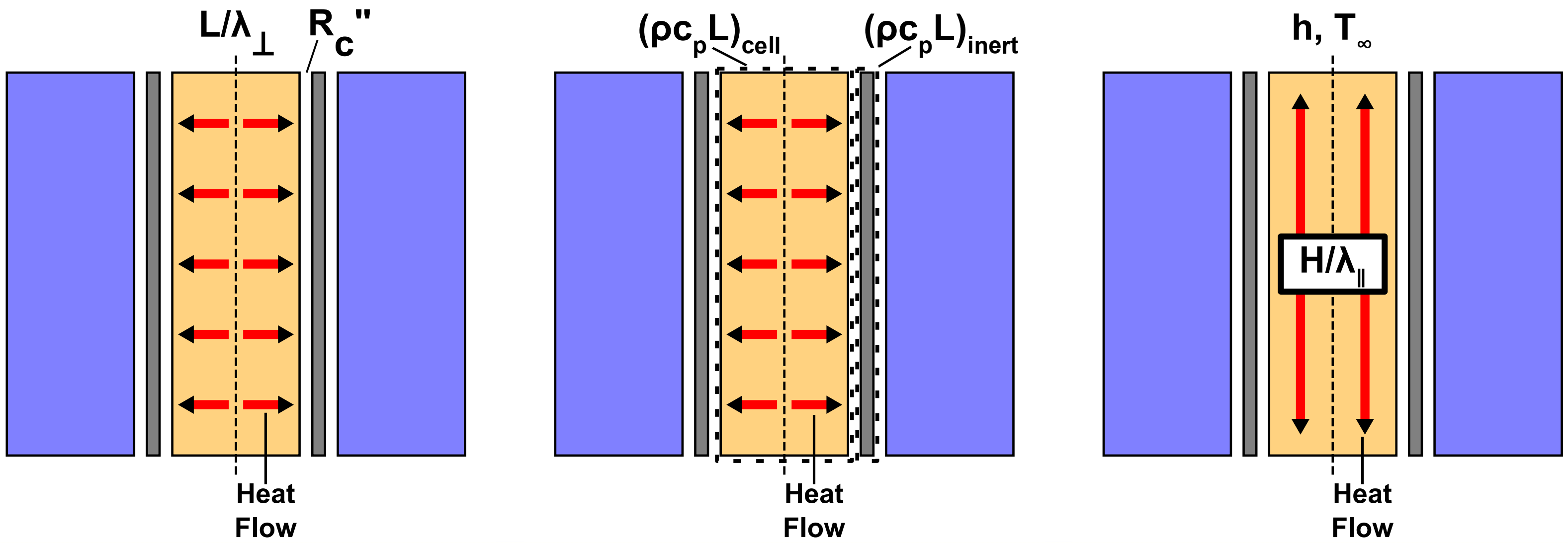




CELL-TO-CELL SCALE PROPAGATION/MITIGATION REGIMES



- Simple model focusing on heat transfer between two cells
- Three non-dimensional parameters can be used to describe heat transfer
  - Conduction resistance
  - Heat capacity ratio
  - External losses
- Thermal runaway assumed when $T_c > T_{onset}$



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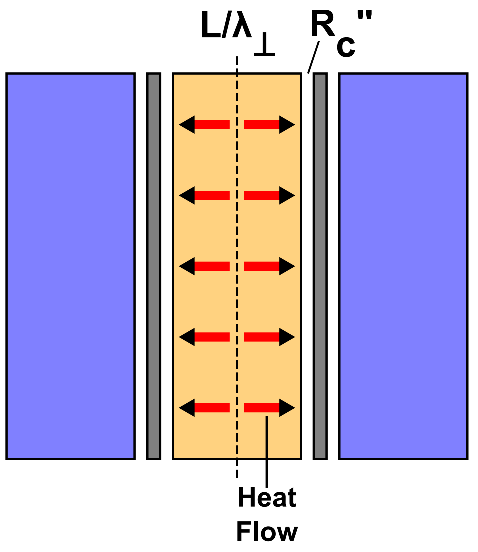
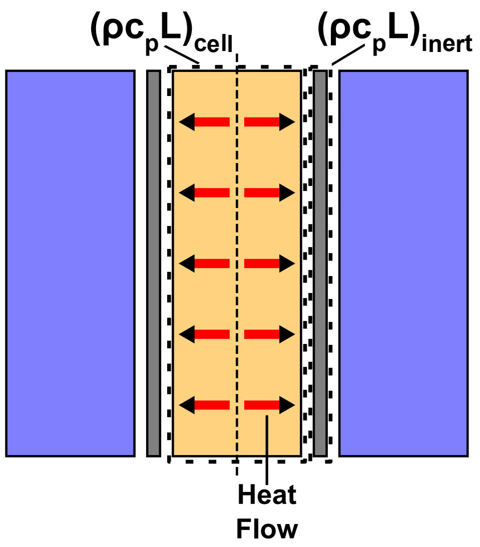
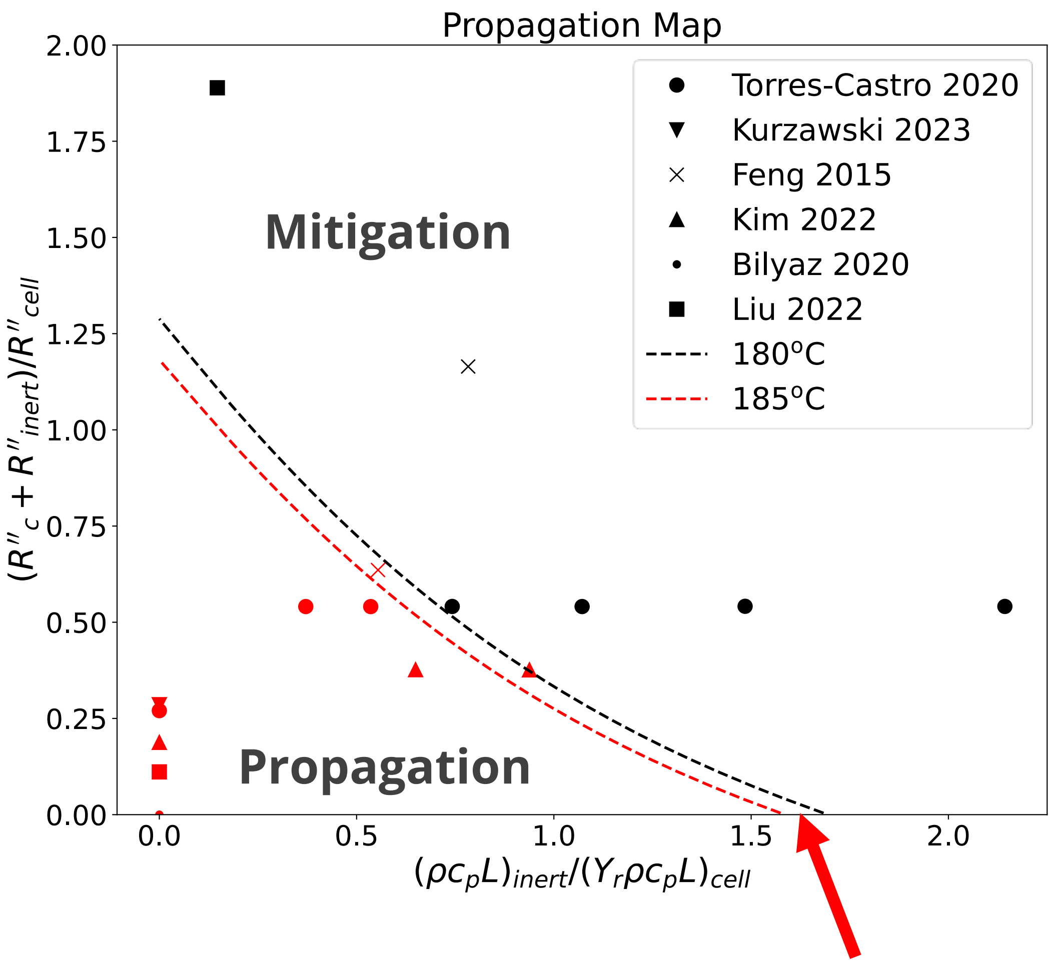






Modeled T_{onset} boundaries

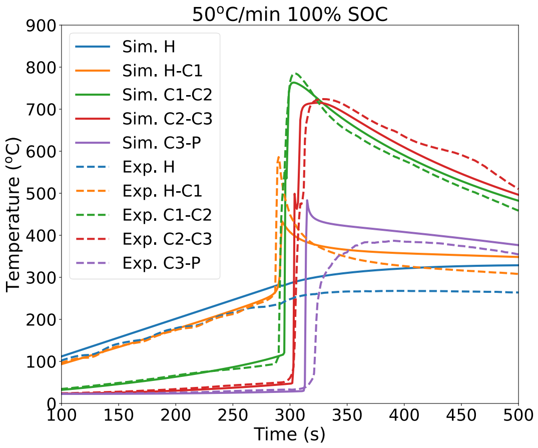
Key features

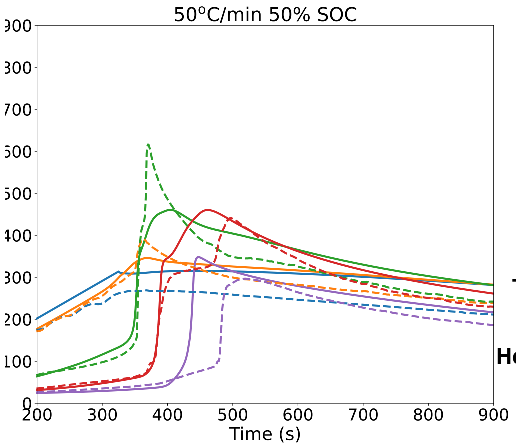
- Assume losses to ambient
- Range of cell sizes with different inter-cell materials
- Vertical axis: ratio of inter-cell resistance to internal resistance
- Horizontal axis: ratio of intercell heat capacity to heat capacity remaining in cell after venting

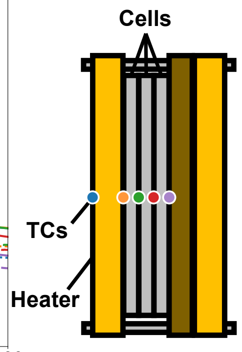
Main uncertainties

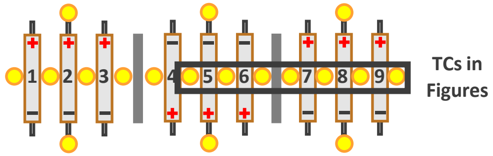
- Mass loss
- Contact resistance

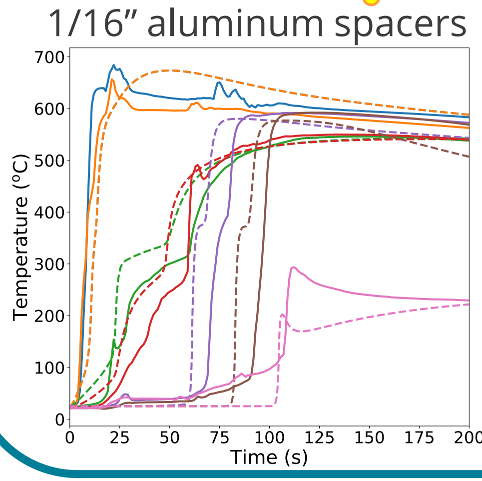
VALIDATION OF PROPAGATION/MITIGATION

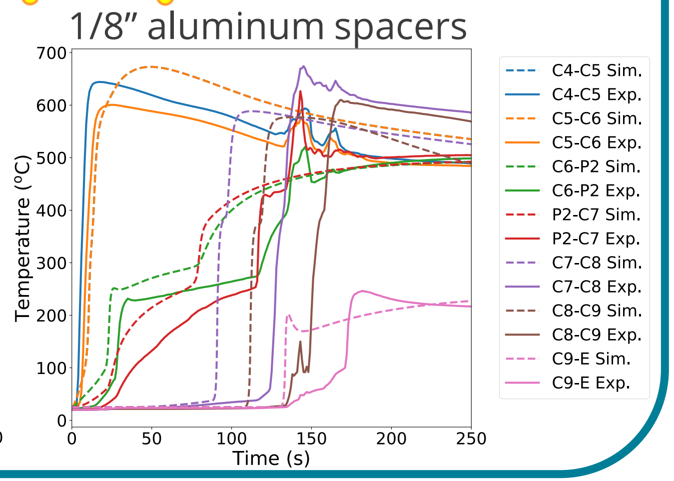


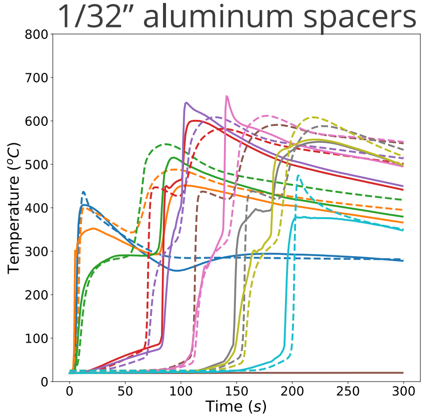


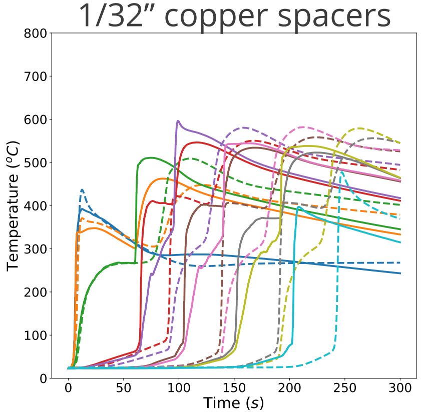


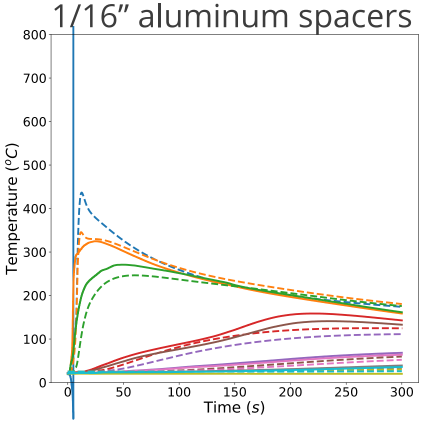


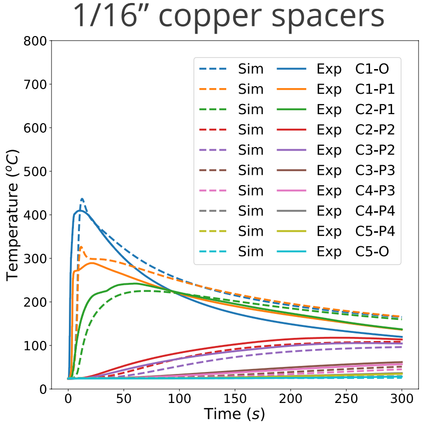


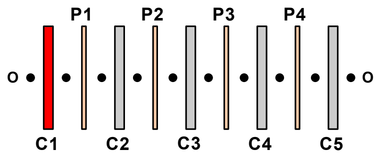








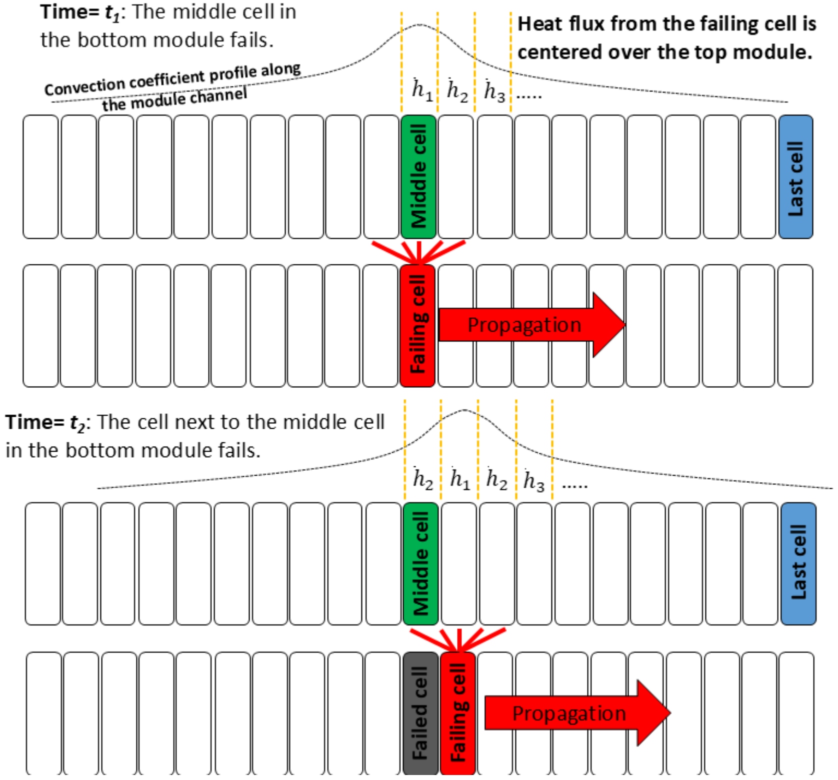




VENT GAS HEAT TRANSFER

- Li-ion batteries undergoing thermal runaway produce hot combustible gases and solid particles that can heat other cells in the system
- Gases impinge directly on the surface above and travel through channels between modules, heating more distant cells.
- Heating from successive failures spreads heat through the system.

Example vent impingement



Lower module to upper module heat transfer from successive vents

Simulations from A. Qatramez, D. Foti, and A. Headley at The University of Memphis

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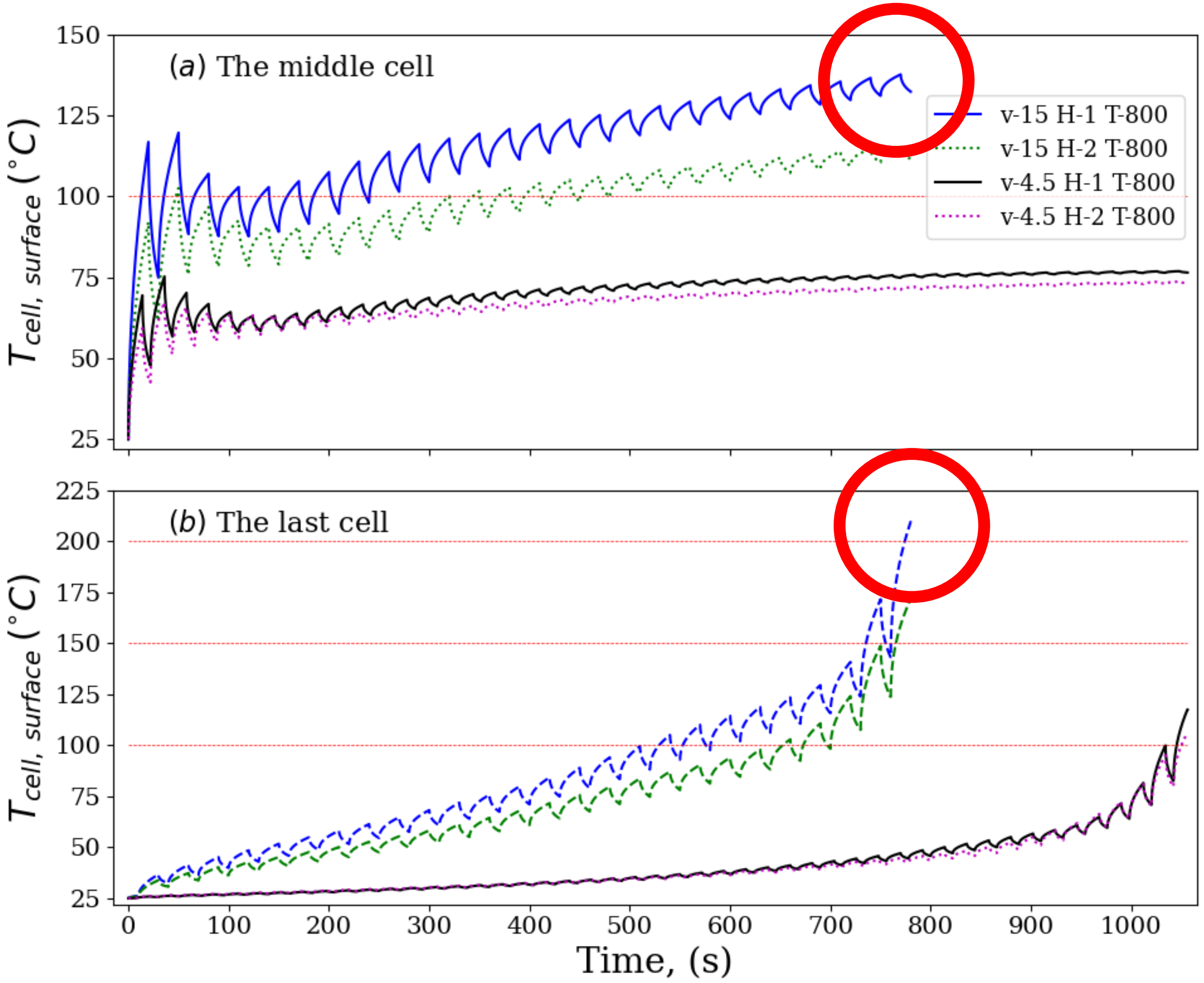


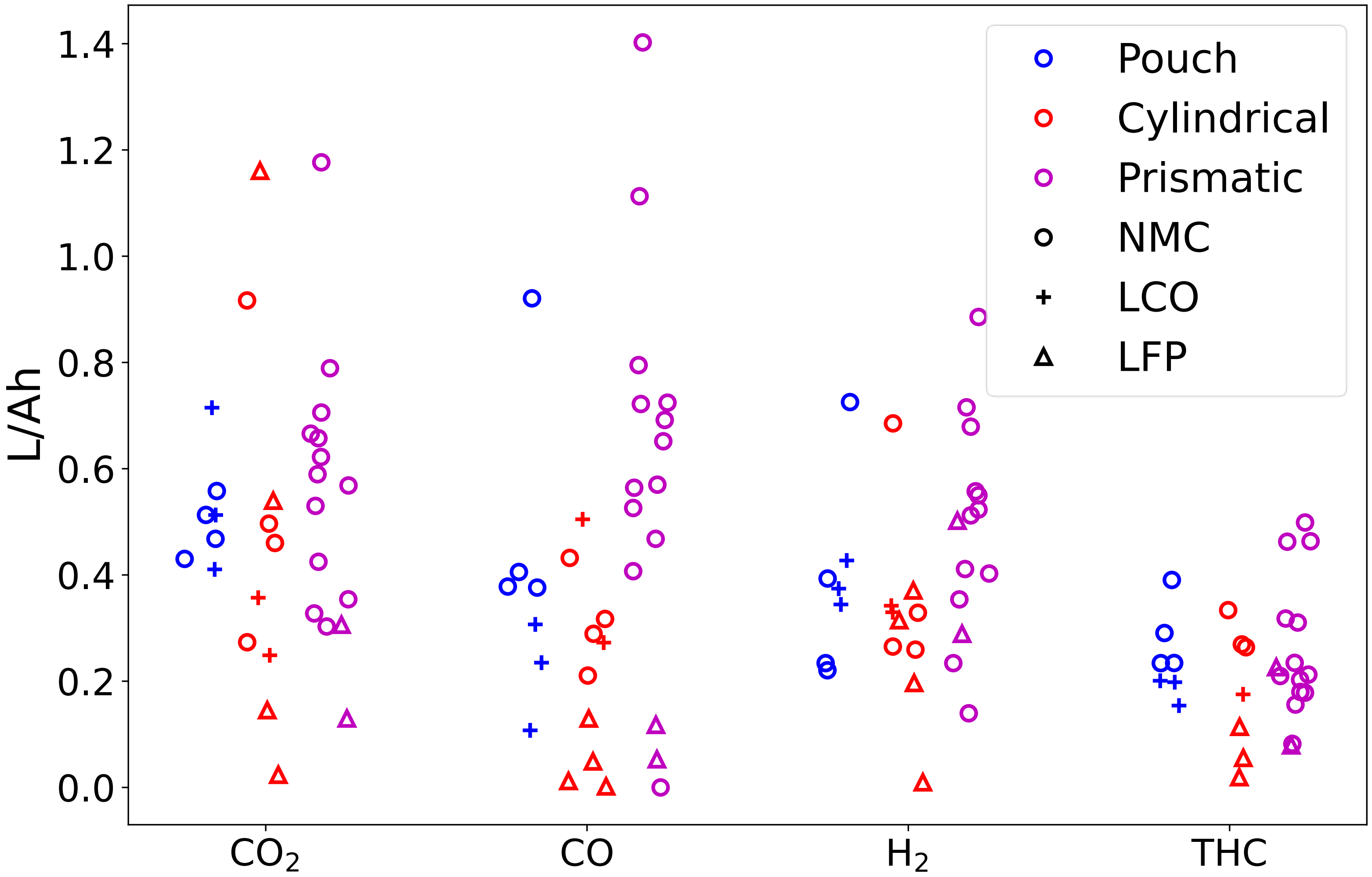
Preheating of the last cell of the upper module results in higher temperatures

Simulations from A. Qatramez, D. Foti, and A. Headley at The University of Memphis

VENT GAS COMPOSITION: LITERATURE DATA

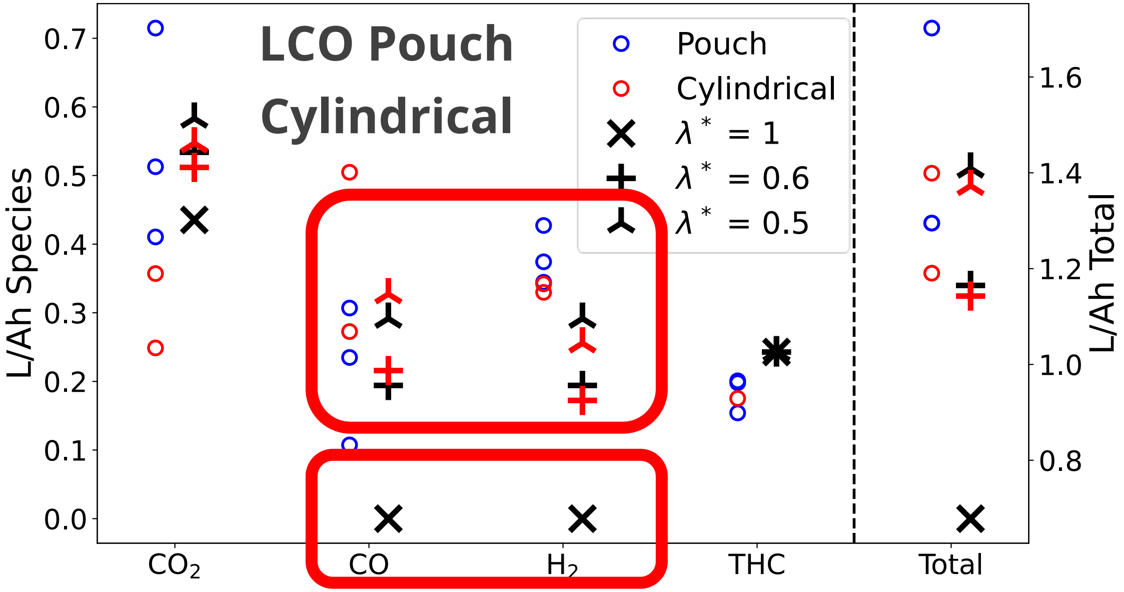
- The vent gas is primarily composed of CO_2, CO, H_2, and hydrocarbons.
- The flammable gases can burn or pose explosion/deflagration hazard.
- Recent studies (Baird et al. 2020 and Bugryniec et al. 2024) have aggregated data from multiple sources.
- A large amount of variability exists in the data even between replicates in the same study.

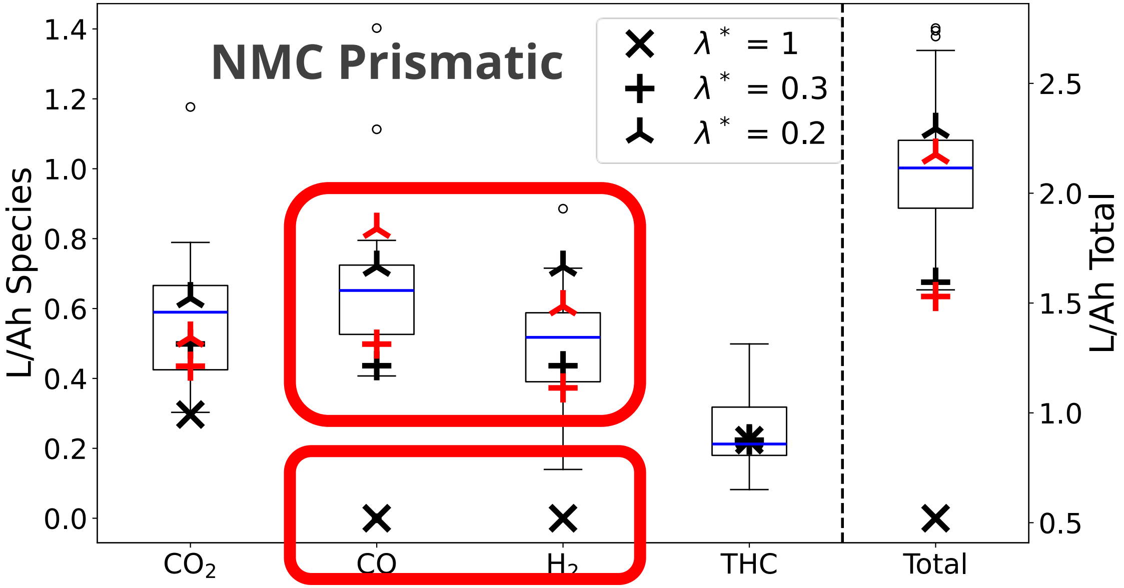
100% SOC cells in inert environments with different abuse methods



Data from Bugryniec et al. 2024 https://doi.org/10.1016/j.est.2024.111288

VENT GAS COMPOSITION: MODELING





- Modeled thermal runaway and gas production for two example cells in LIM1TR software.
- Full oxidation of ethylene carbonate (EC) only produces CO_2 and water vapor.

$$5MO_2 + (CH_2O)_2CO \rightarrow 5MO + 3CO_2 + 2H_2O$$

- Partial oxidation of EC

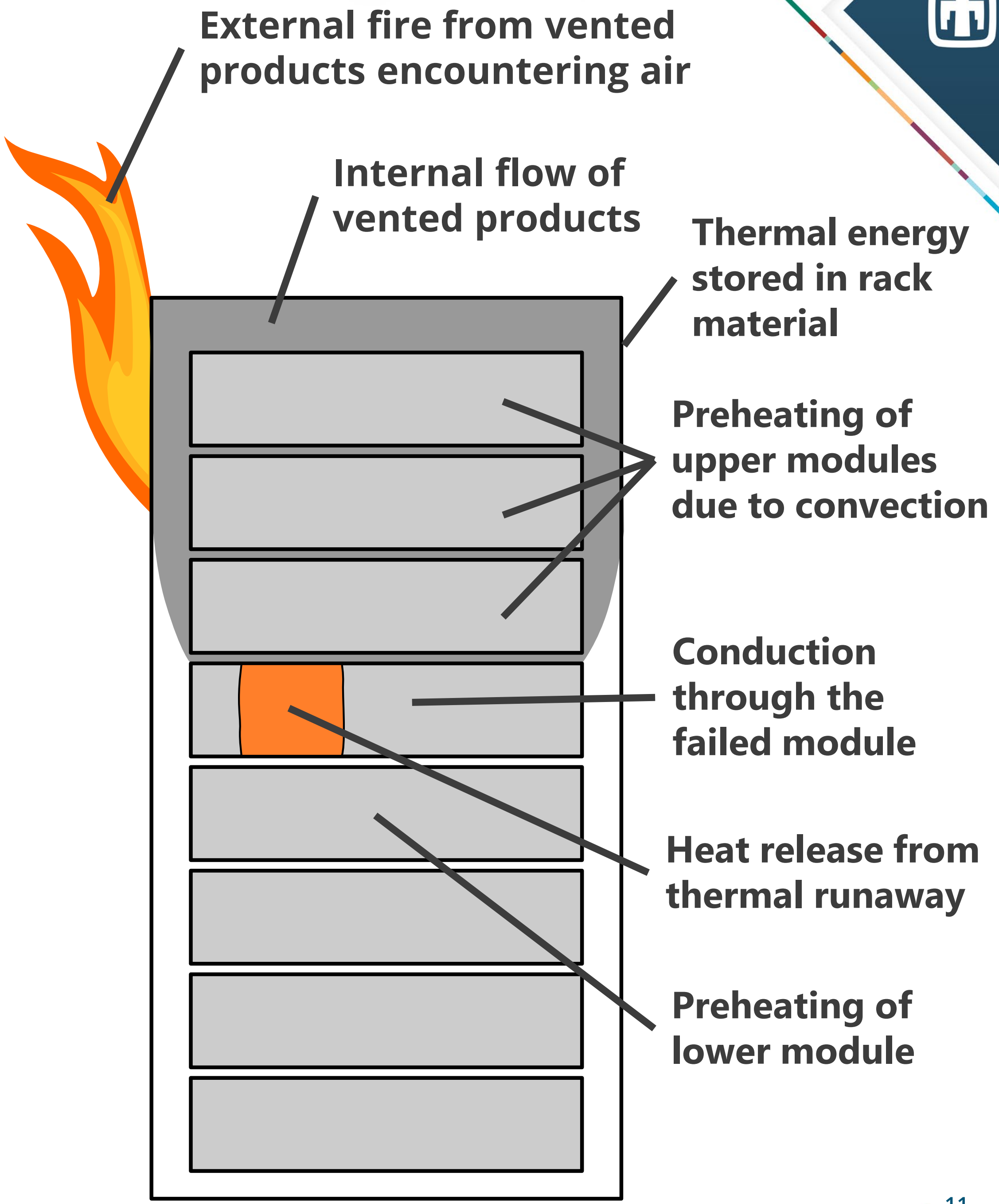
$$5MO_2 + \phi(CH_2O)_2CO \rightarrow 5MO + aCO_2 + bCO + cH_2O + dH_2$$

- Two closure methods for partial oxidation: linear closure (black symbols) and water-gas shift closure (red symbols).
- The inclusion of cathode partial oxidation improves gas predictions, and ongoing work is focused on contributions from the anode.

HEAT TRANSFER AT THE RACK SCALE

Modeling challenges at the rack scale:

- **Variability in design**: enclosed/open shelves, presence of wiring, ventilation pathways, passive/active cooling.
- **Uncertainties**: thermal contact resistances, cell heat release, dynamical ventilation pathways, pressure loss coefficients for gas accumulation.
- **Multi-physics coupling**: turbulence, combustion, phase change (e.g., plastic/aluminum melting), chemistry.
- **Sparse availability of test data**: testing at these scales are dangerous, expensive, and generally involves proprietary information



RACK MODEL

Description: 2-D sims with Sandia's Sierra/Fuego CFD code to simulate battery venting. A RANS turbulence model and EDC combustion model are used. Statistics are taken after flow becomes (statistically) stationary.

Parameter list:

- Module width: 80 cm
- Module height: 10 cm
- Opening width: 10 cm
- Channel height: 2 cm
- Vent width: 1 cm
- Vent velocities: 1, 2, ..., 25 m/s
- Vent module: 1, 3, 5
- Vent temperature: 800, 1200 K
- Air temperature: 300 K

Roughly equivalent to LFP pouch cell

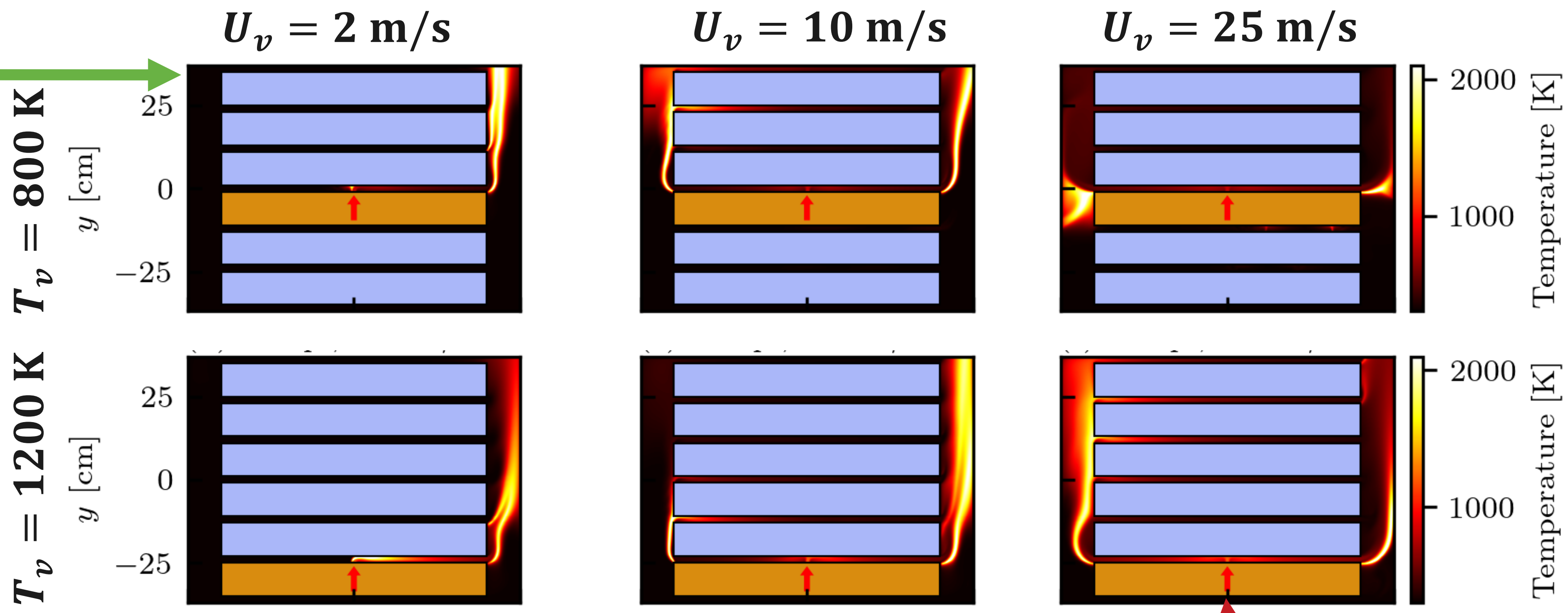


Figure showing time-average temperature fields for different vent velocities and temperatures

Approaching equivalence of NMC prismatic cell

VENT GAS FLOW AND HEAT TRANSFER

Key findings:

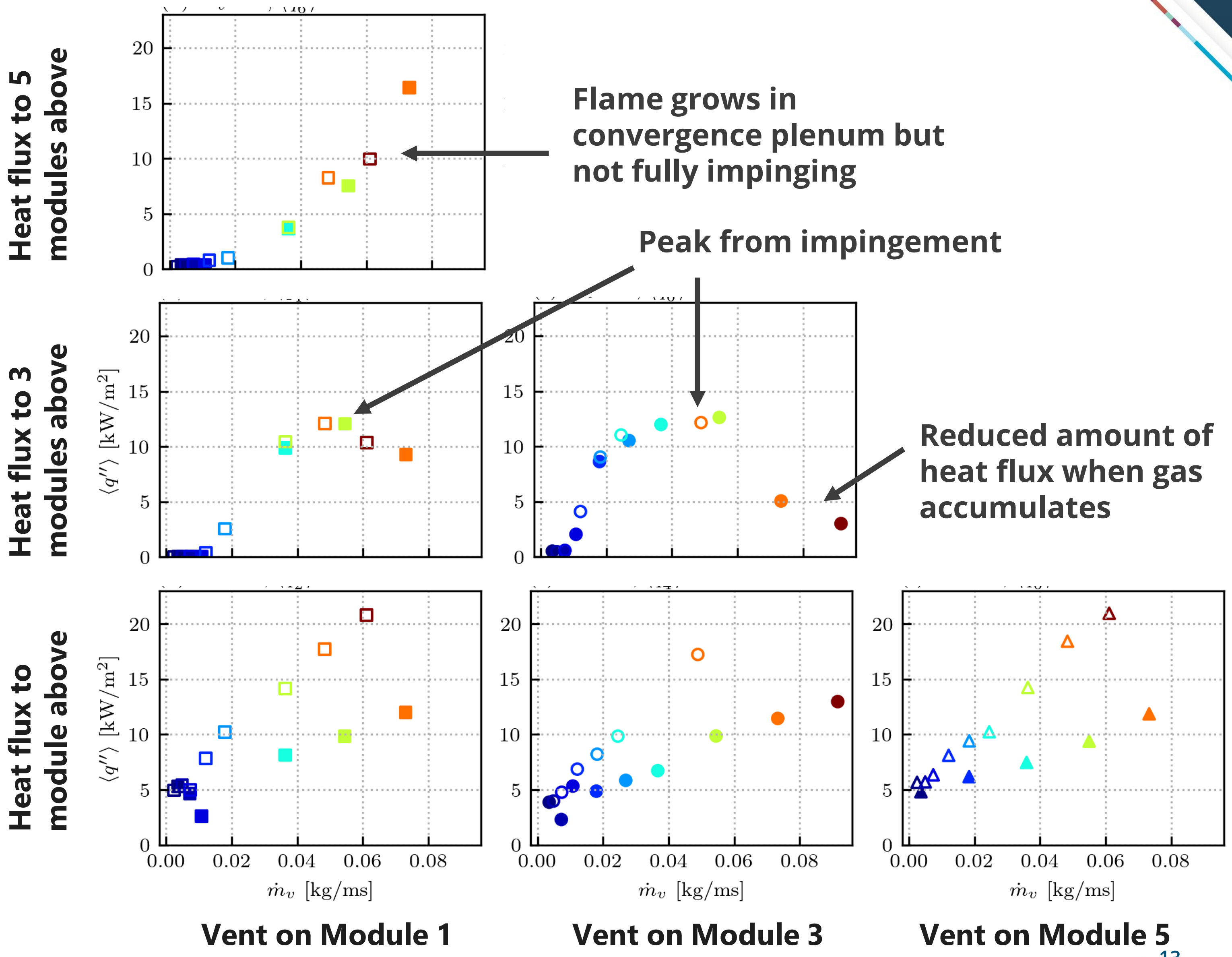
- Heat flux to the module above venting (bottom row) scales according to jet impingement physics
- Heat flux to non-adjacent modules peaks when flame impinges on the module and remains non-zero during hot gas accumulation.

<u>Legend for images</u>

Color: blue to red = increasing velocity

Symbol: module number

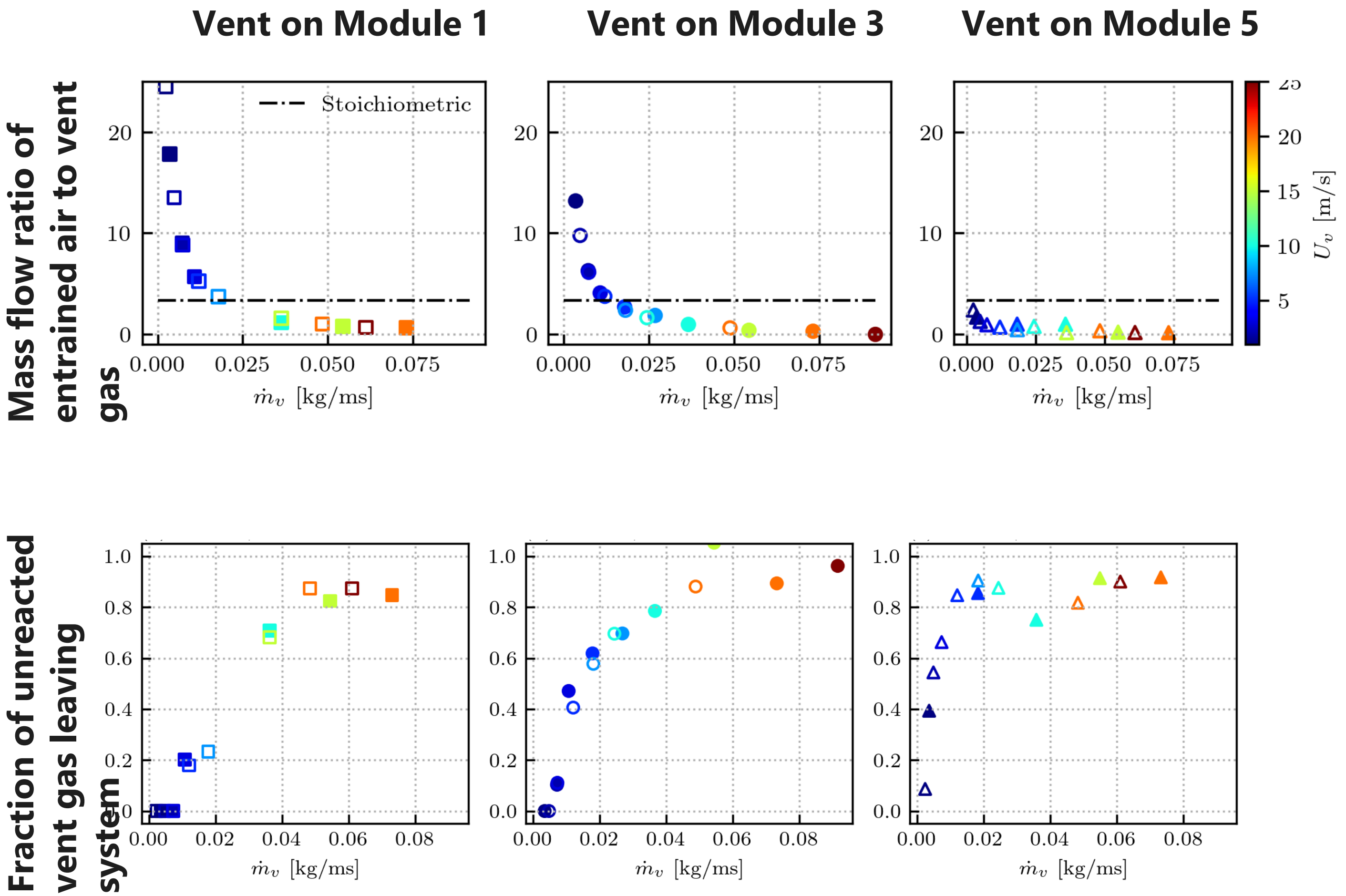
Fill: open = higher vent temperature



VENT GAS FLOW AND HEAT TRANSFER

Key findings:

- More air entrainment when the vent is near the bottom and released slowly to generate large buoyant force relative to momentum
- Under most realistic conditions, vent gas leaves ESS unreacted. Resulting in heat release outside of rack endangering neighboring racks.
- Unreacted vent gases mixed with entrained air near stoichiometric conditions pose a greater ignition/deflagration hazard.



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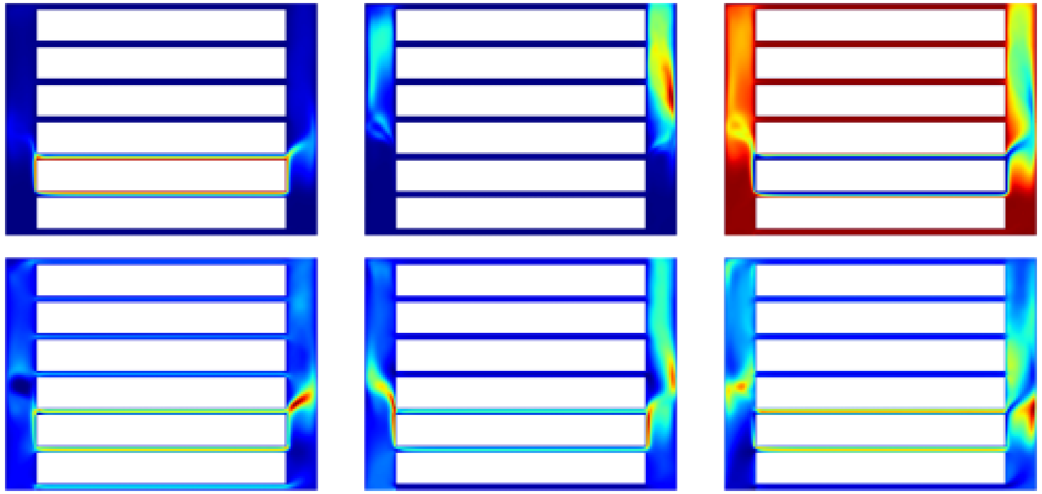
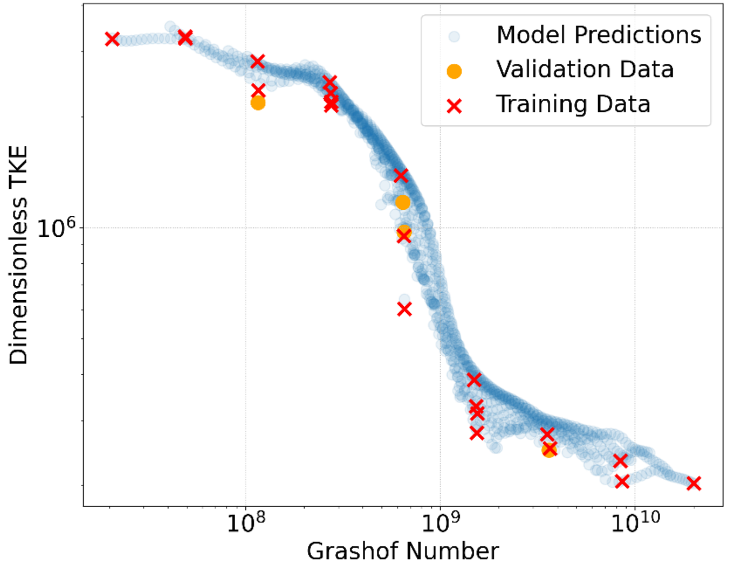
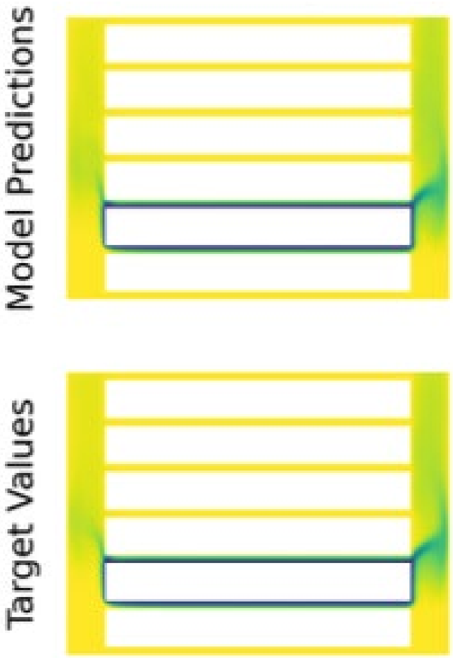
MACHINE LEARNING APPROACH

- Use *structure-preserving* reduced-order modeling methods to *learn* a reduced finite element basis and a nonlinear conservation law using simulation data. Creates physics-conserving model by *construction*.
- The reduced-order model can:
  - Feedback into cell-to-cell propagation (e.g., heat flux)
  - Build control algorithms for active mitigation
  - Include physics-conserving properties by construction



Reduce simulations of millions of elements to only 6 coarse elements, allows <u>real-time evaluation</u> speeds

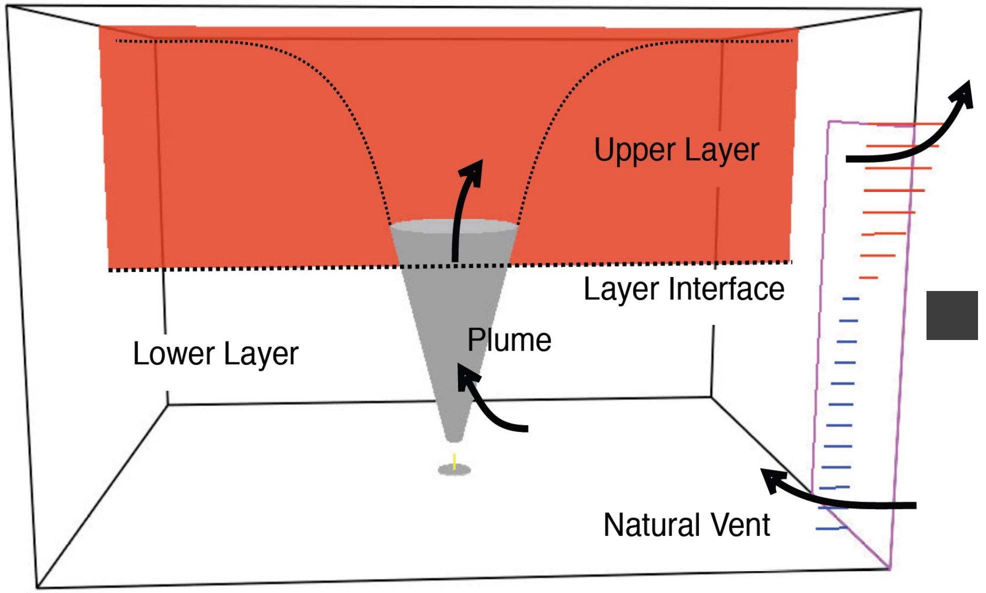




Excellent accuracy shown using turbulent kinetic energy (heat transfer, left) and field reconstructions (right)

HEAT TRANSFER BEYOND THE ORIGINATING RACK

- CFD at the room scale is computationally expensive, inhibiting exploration of large parameter spaces
- Correlations and network models offer means of exploring parameters, but these models need inputs from the rack scale models

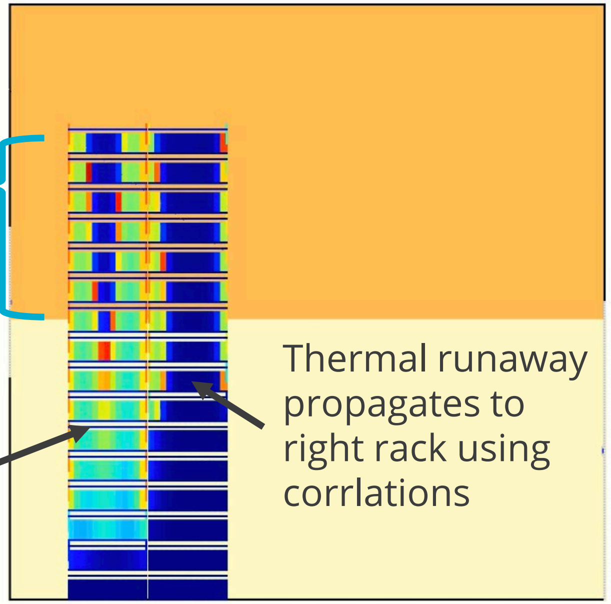


Components of mass and enthalpy entering or leaving a control volume

**Source: CFAST Technical Reference Guide Version 7*

Upper modules are surrounded by upper gas layer

Thermal runaway initiated in left rack and propagates to modules within rack

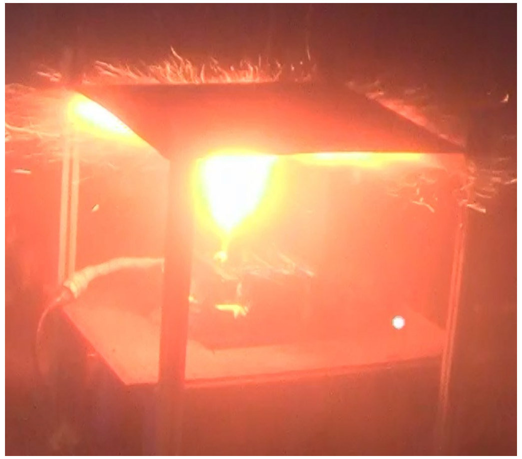


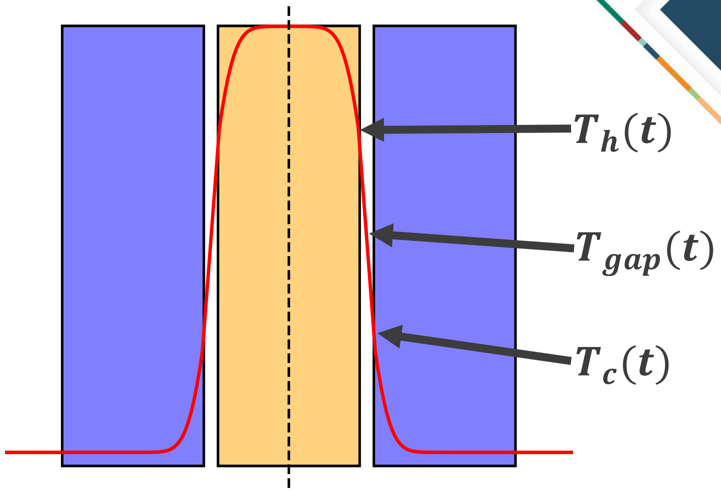
Upper gas layer size is dictated by cell level gas composition and release rate within rack(s)

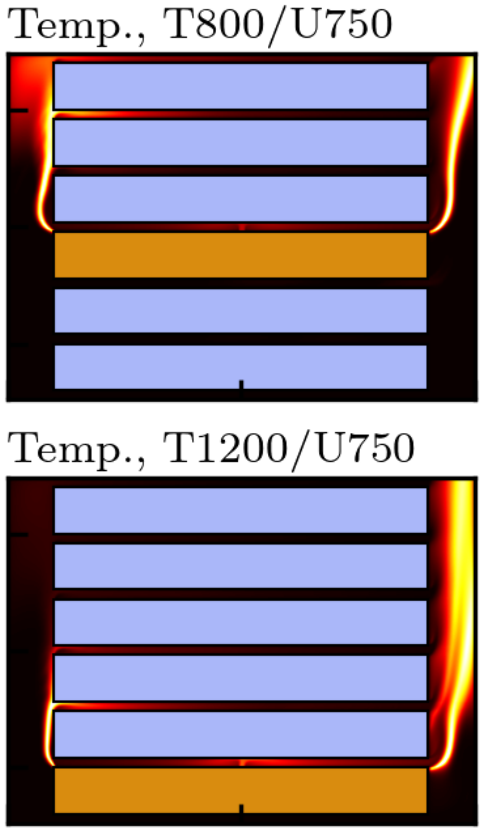
- Continuation of testing campaigns better grounds models in physical reality

SUMMARY

- A range of modeling tools are needed to predict thermal runaway at different scales.
- Models feed into each other, from cell-level heat and gas release up to room-scale fire effects.
- We seek to balance accuracy and computational complexity to explore a range of scenarios while validating predictions against along the way.







ACKNOWLEDGEMENTS

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We would like to thank our collaborators at the University of Memphis and the battery safety thrust area at Sandia.