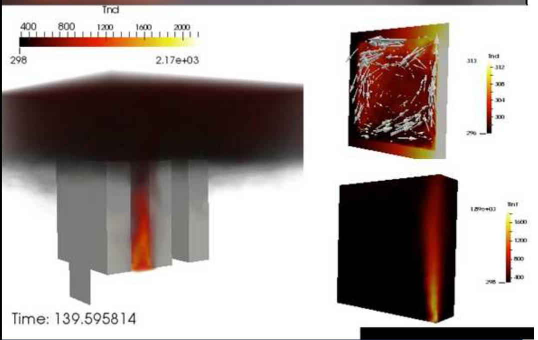
SAND2015-3943C



Thermal Runaway of Lithium-Ion Batteries and Hazards of Abnormal Thermal Environments

John Hewson, Stefan Domino
Engineering Sciences Center
Sandia National Laboratories

US Sections Section Combustion Institute Meeting
May 19, 2015

Sandia National Laboratories

Exceptional service in the national interest

U.S. DEPARTMENT OF ENERGY

National Nuclear Security Administration

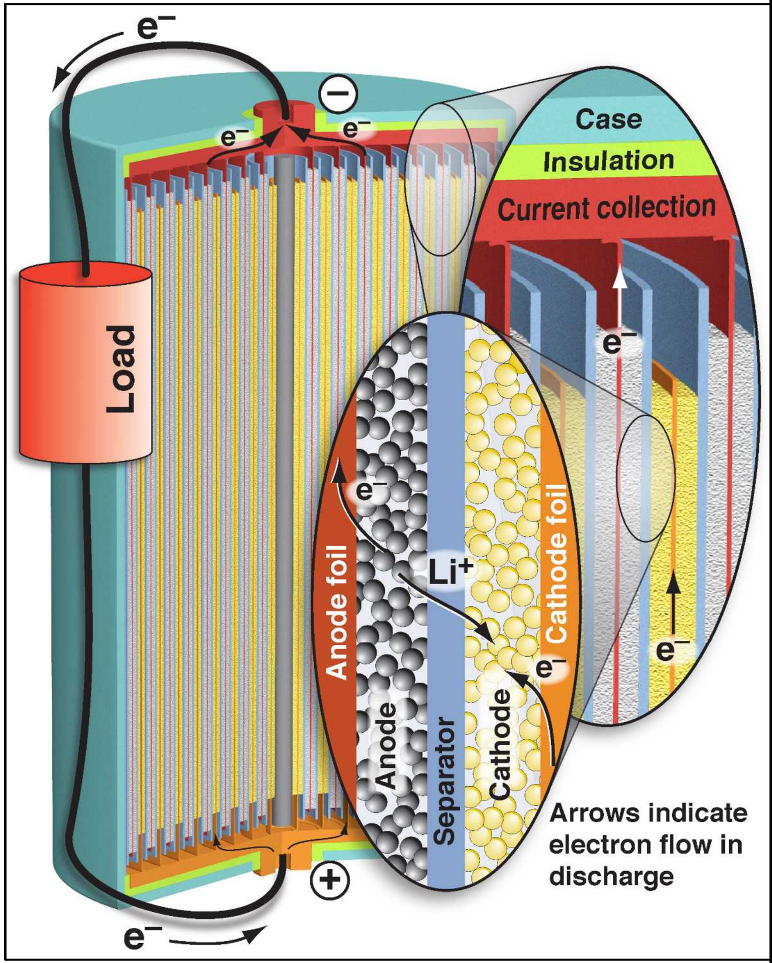
Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Energy Storage Safety/Reliability Issues Have Impact Across Multiple Application Sectors

Sandia National Laboratories

Motivation

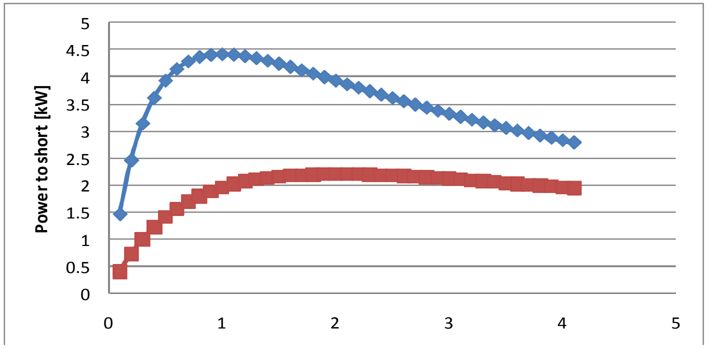
- Energy storage in electrochemical systems (batteries) is increasingly prevalent.
  - Energy storage facilities 3kWh to MWh scale.
  - Vehicle battery systems comparable to a 'gas tank' (50 kWh)
  - Laptops, etc., with 60 Wh.
- Potential hazards associated with stored energy couple with inexperience regarding safety and mitigation practices.
  - What are ignition characteristics?
  - What are hazards, both thermal and chemical?
  - What mitigation is appropriate?



- Safety characteristics need to be evaluated; standards and best-practices need to be developed.

Unique aspects of batteries in fire environments

- Stored battery energy is available to generate heat—essentially a premixed fuel and oxidizer in a pressure vessel.
- External heating, short circuits, overcharging can all destabilize stored energy.
- Beyond stored energy, chemical energy available from flammable electrolytes and packaging.
- Internal or external short circuits can lead to ohmic heating of battery (I^2R)
  - Nail penetration, dendrite formation, crush, etc.
  - Parallel versus series cells.



V_{OC} = 4.2 V; R_{cell} = 1 mΩ (blue) and R_{cell} = 2 mΩ (red)

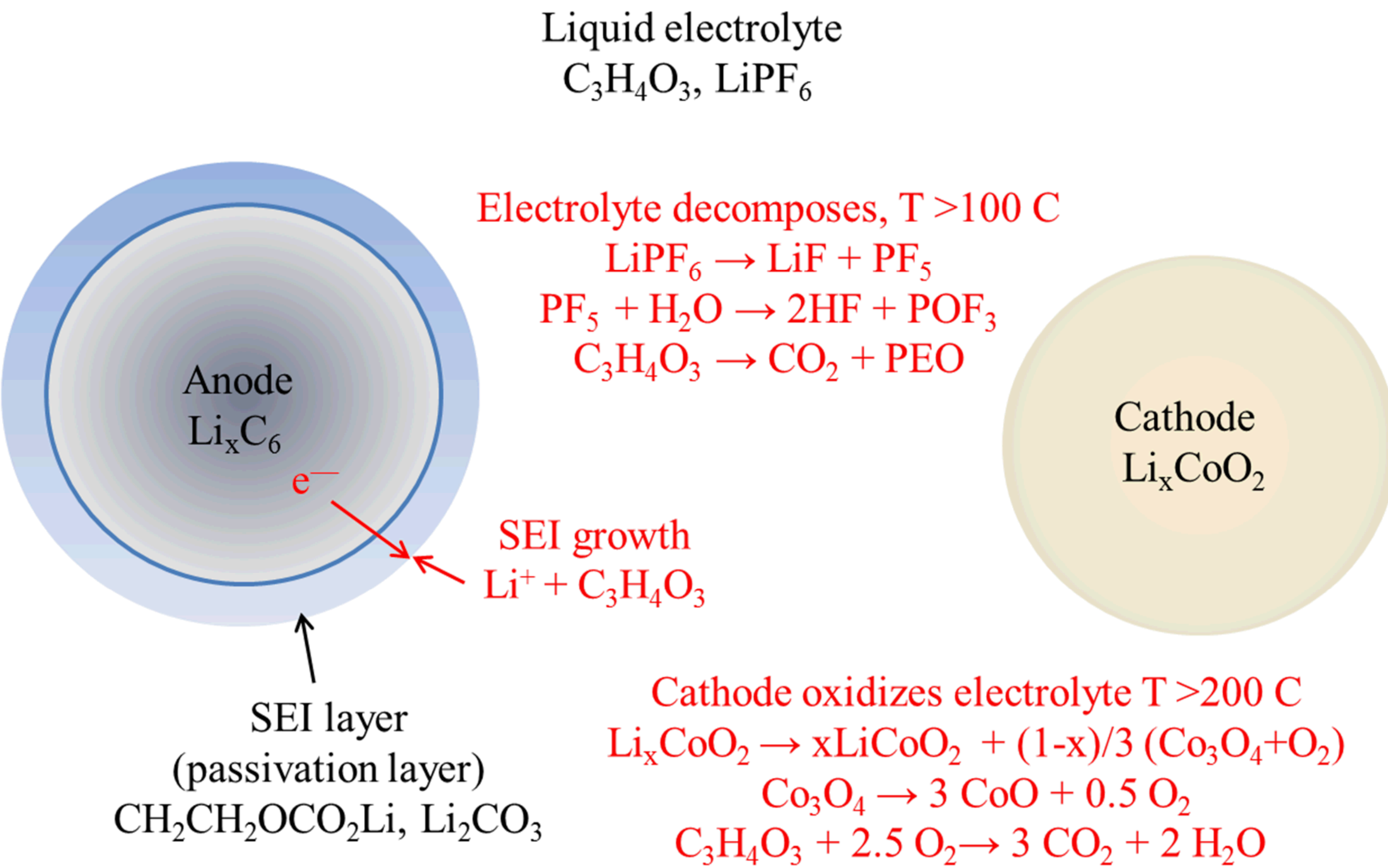
Power associated with internal cell resistance:

$$P_{cell} = \left(V_{OC}\right)^2 \frac{R_{cell}}{\left(R_{cell} + R_{short}\right)^2}$$

Power associated with short circuit:

$$P_{short} = \left(V_{OC}\right)^2 \frac{R_{short}}{\left(R_{cell} + R_{short}\right)^2}$$

Some sources of energy in a Li-Ion battery

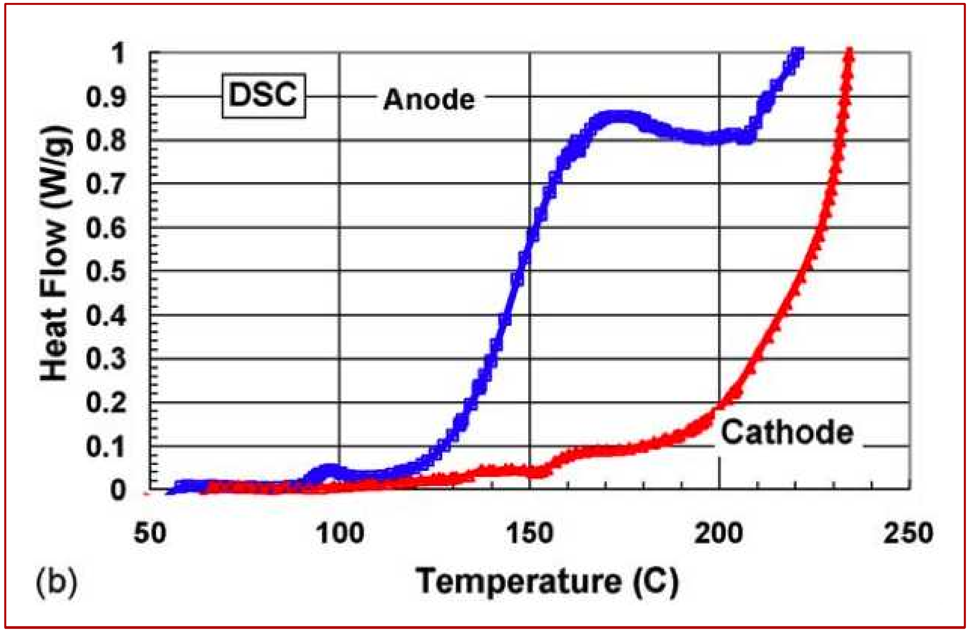


Some sources of energy in a Li-Ion battery

- Nominal heat release and and temperature ranges for internal degradation reactions (Hatchard and Dahn, 2001)
  - SEI decomposition: 257 kJ/kg (100-150 C)
  - Anode-electrolyte reaction: 1714 kJ/kg (150-250 C)
  - Cathode-electrolyte reaction: 4000 kJ/kg (200-250 C)
    - $Li_{0.5}CoO_2 + 0.1\ C_3H_4O_3$ -> $0.5\ LiCoO_2 + 0.17\ Co_3O_4 + 0.3\ CO_2 + 0.2\ H_2O$
  - Electrolyte decomposition: 155 kJ/kg (250-300 C)
  - Energy from short circuit: 300 – 900 kJ/kg (full battery)

- Hydrocarbon oxidation – electrolytes
  - Electrolyte combustion (with O2): 6,800 kJ/kg
  - Compare gasoline-like fuels: 41,000 kJ/kg

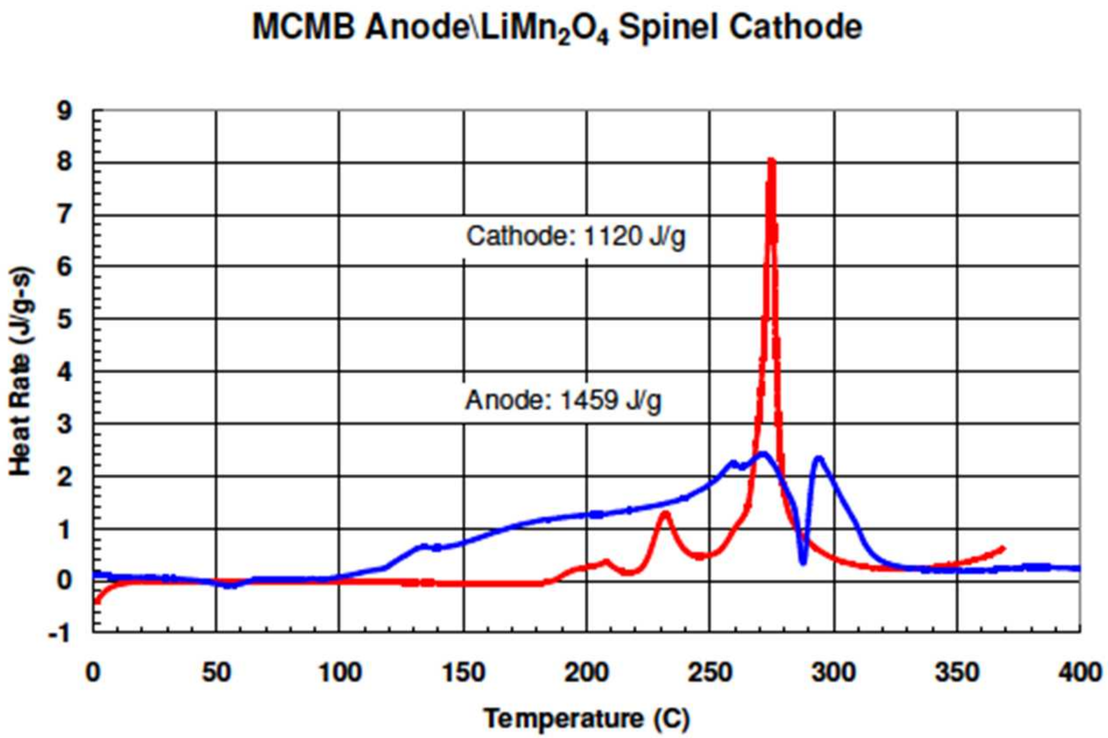
Thermal runaway is associated with anode reactions followed by cathode reactions



Abraham et al. J Pow Sources 161, 648 (2006)

- DSC results suggest that the first step involved in thermal abuse is the breakdown of the SEI layer, exposing Li/C to the solvent.
- Further heating leads to oxygen release from cathode and reaction with electrolyte.

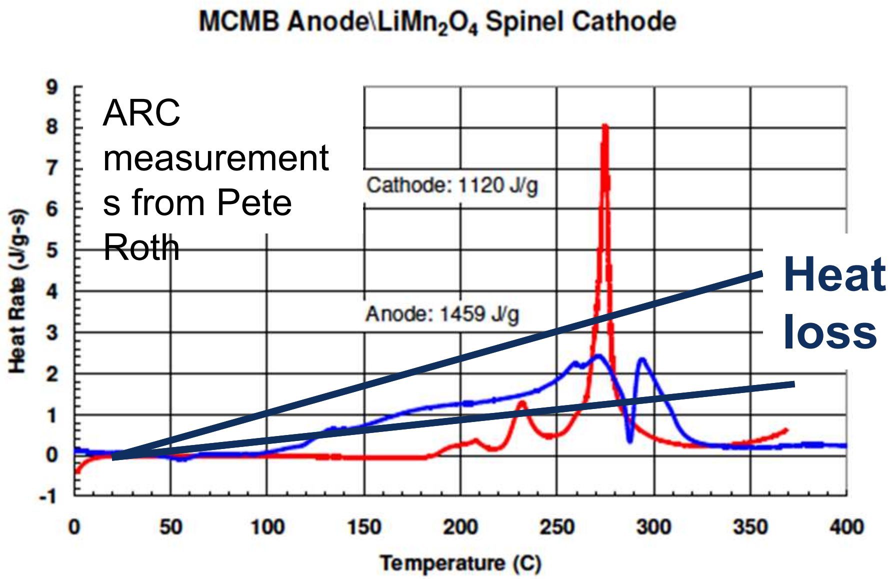
Thermal runaway is associated with anode reactions followed by cathode reactions



ARC measurements from Pete Roth

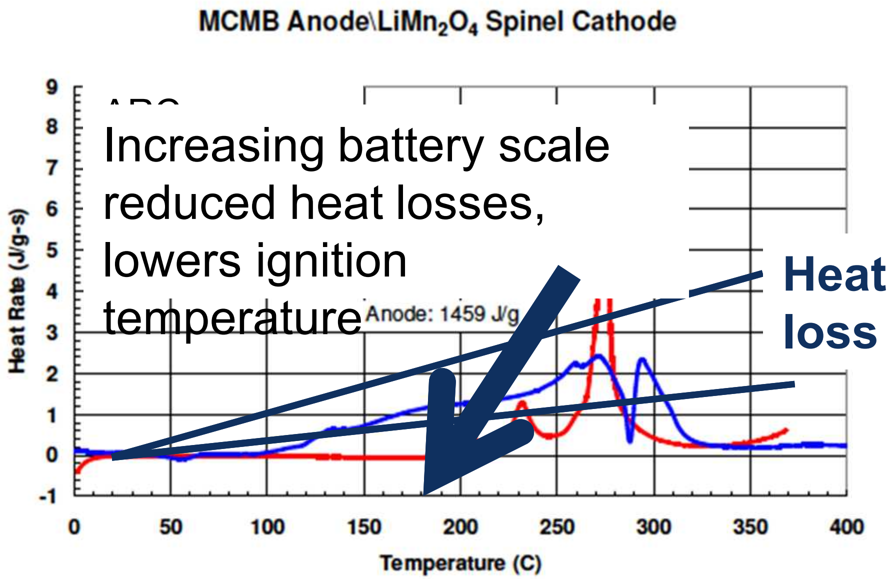
- DSC results suggest that the first step involved in thermal abuse is the breakdown of the SEI layer, exposing Li/C to the solvent.
- Further heating leads to oxygen release from cathode and reaction with electrolyte.

Thermal runaway occurs if heat release exceeds heat losses



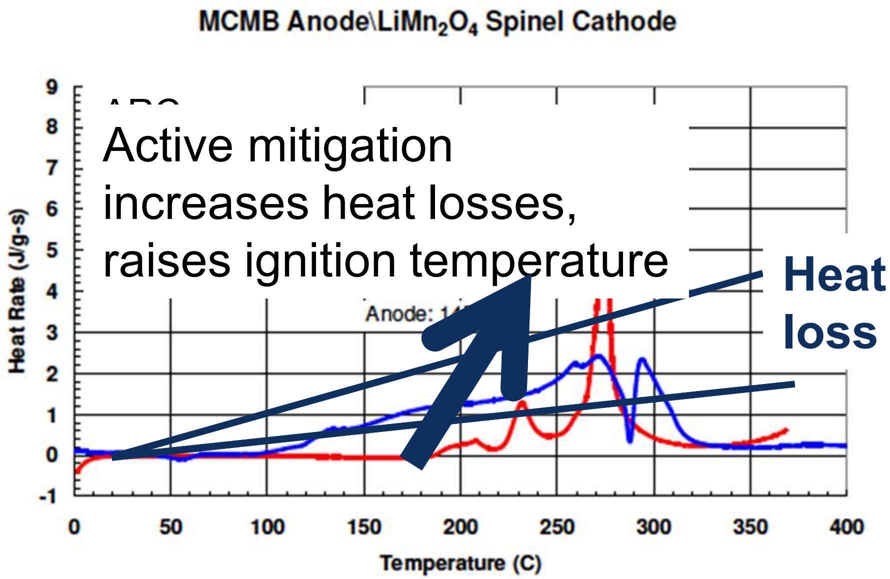
- Increasing battery scale reduces heat losses, lower ignition temperature
- Active suppression/mitigation can increase heat losses, raise ignition temperature.
- Some low temperature degradation should be detectable.

Thermal runaway occurs if heat release exceeds heat losses



- Increasing battery scale reduces heat losses, lower ignition temperature
- Active suppression/mitigation can increase heat losses, raise ignition temperature.
- Some low temperature degradation should be detectable.

Thermal runaway occurs if heat release exceeds heat losses

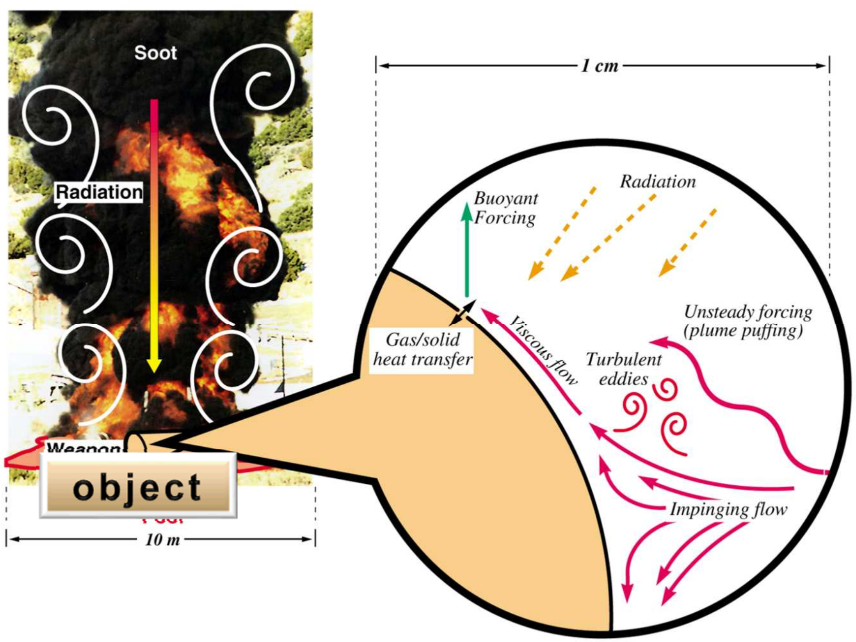


- Increasing battery scale reduces heat losses, lower ignition temperature
- Active suppression/mitigation can increase heat losses, raise ignition temperature.
- Some low temperature degradation should be detectable.

Understanding facility-scale hazards using CFD

Important physics:

- Turbulent fluid mechanics including buoyant flow, wall heat transfer.
- Reacting flow: gas-phase, sprays, particle oxidation/reduction and other interphase reactions.
- Conjugate heat transfer including participating media radiation.



Heat transfer mechanisms in a fire

- The simulation tool predicts the thermal environment that balances cell internal heat release and decomposition kinetics.
  - Opens some parameter space to exploration.
  - Identifies sensitivities to heat-dissipation strategies, insulation, ventilation, etc.

Stationary storage application

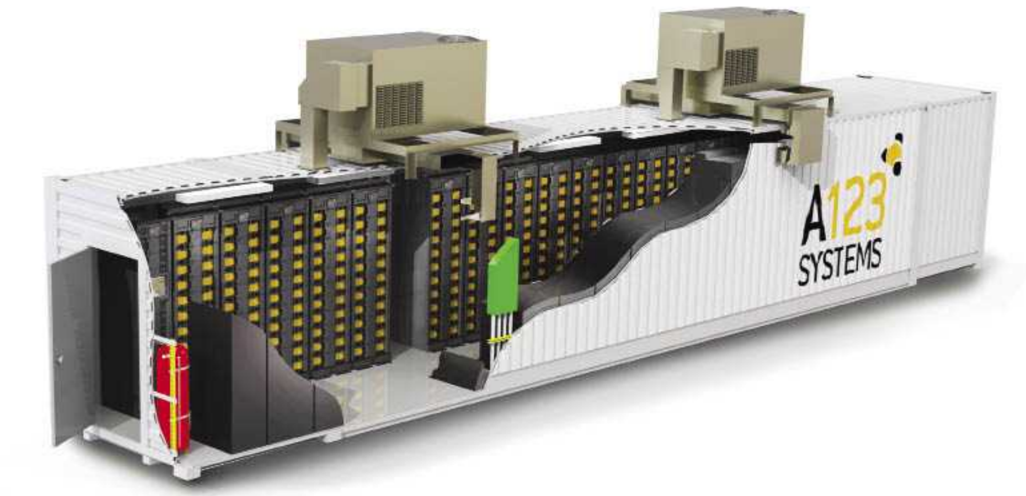
Use Case: Hawaii Lead Acid Batter System on Fire

- Racks of lead acid batteries and power conditioning system inside the building
- No emergency response (Hawaii is a closed water system)

- In what context could we imaging a computational capability being useful?

Relevant geometries

Sandia National Laboratories



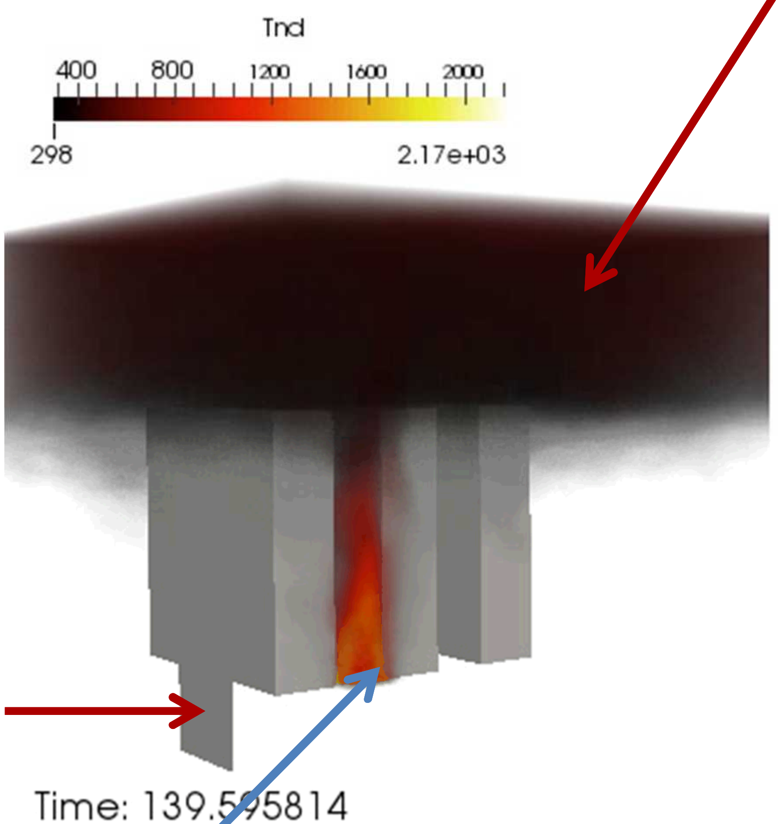
Plug-and-play Lithium Ion trailer

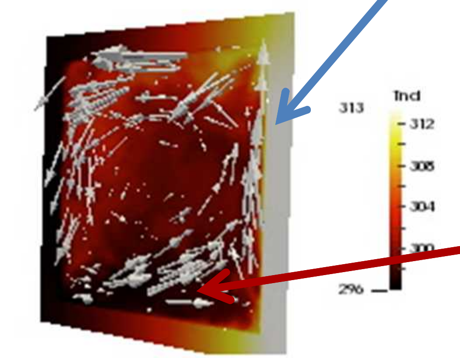
racks of batteries

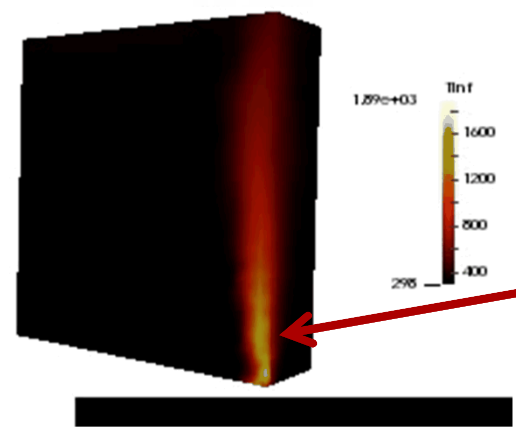
power conditioning system

Lead acid Alaska facility designed to replace back-up diesel

Applying Sierra codes to battery fire scenario







Ventilation (flow out)

Object heat up

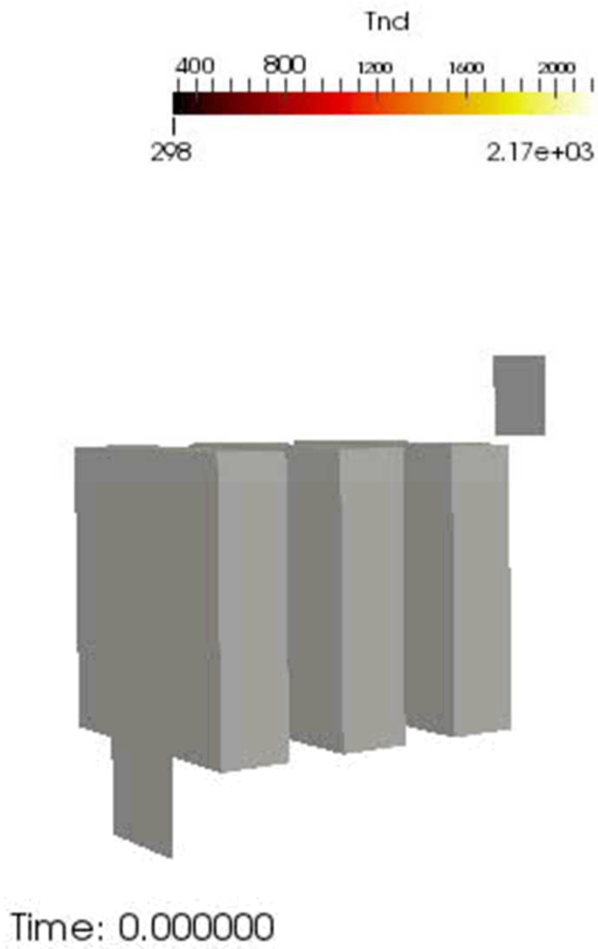
Inner pressurizing Fluid (buoyant)

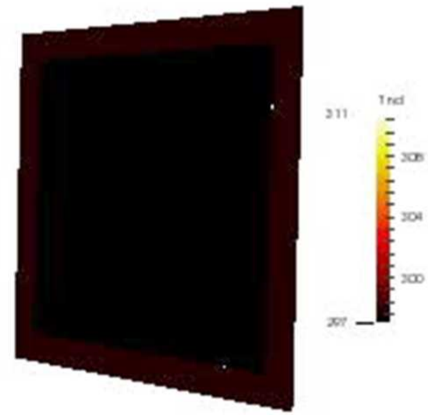
Outer Heat flux

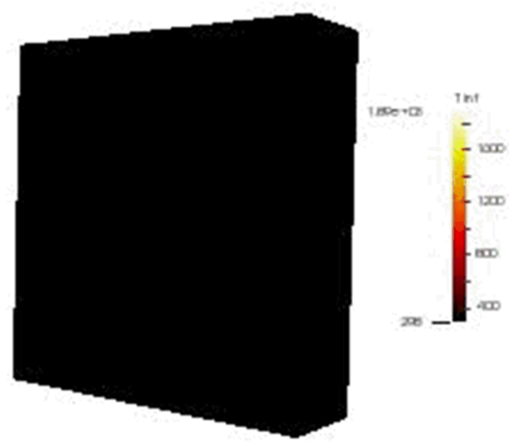
Ventilation (flow in)

Fire modeled as a combustible hydrocarbon

Ventilation effect on fire plume dynamics (1/3)

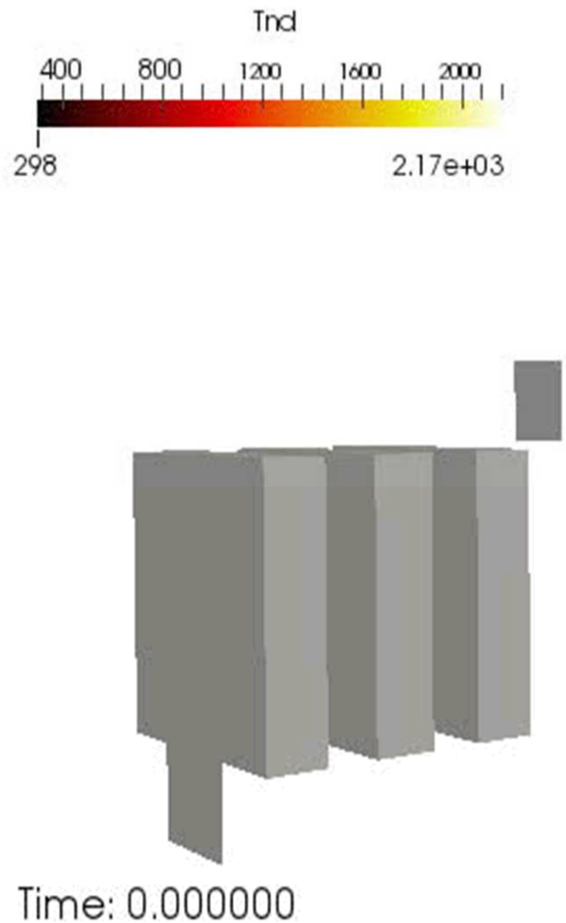


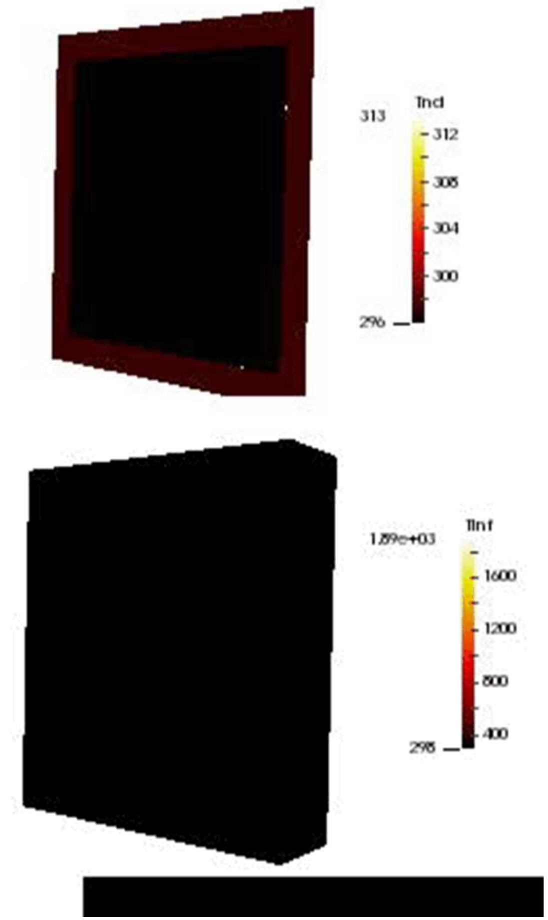




No Ventilation

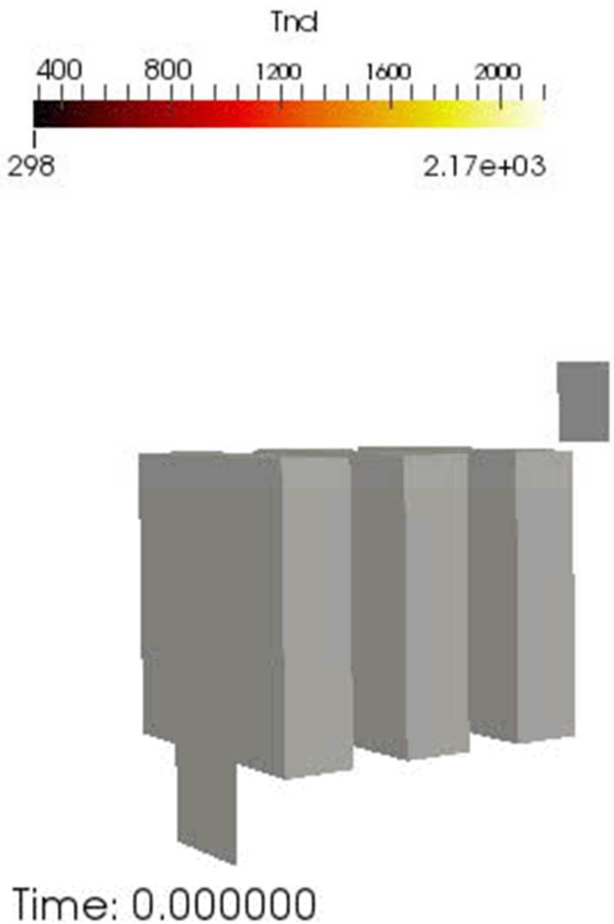
Ventilation effect on fire plume dynamics (2/3)

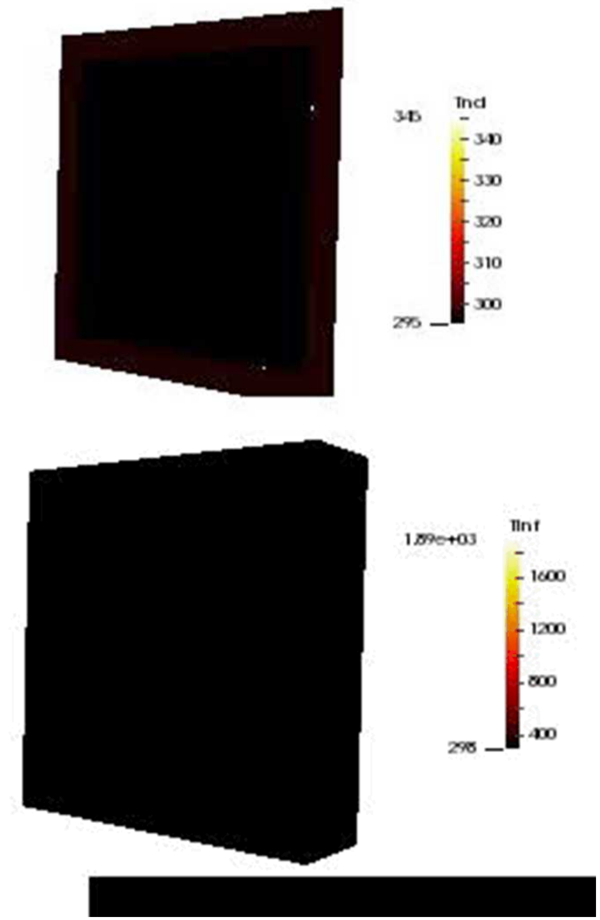




Ventilation is 1 m/s

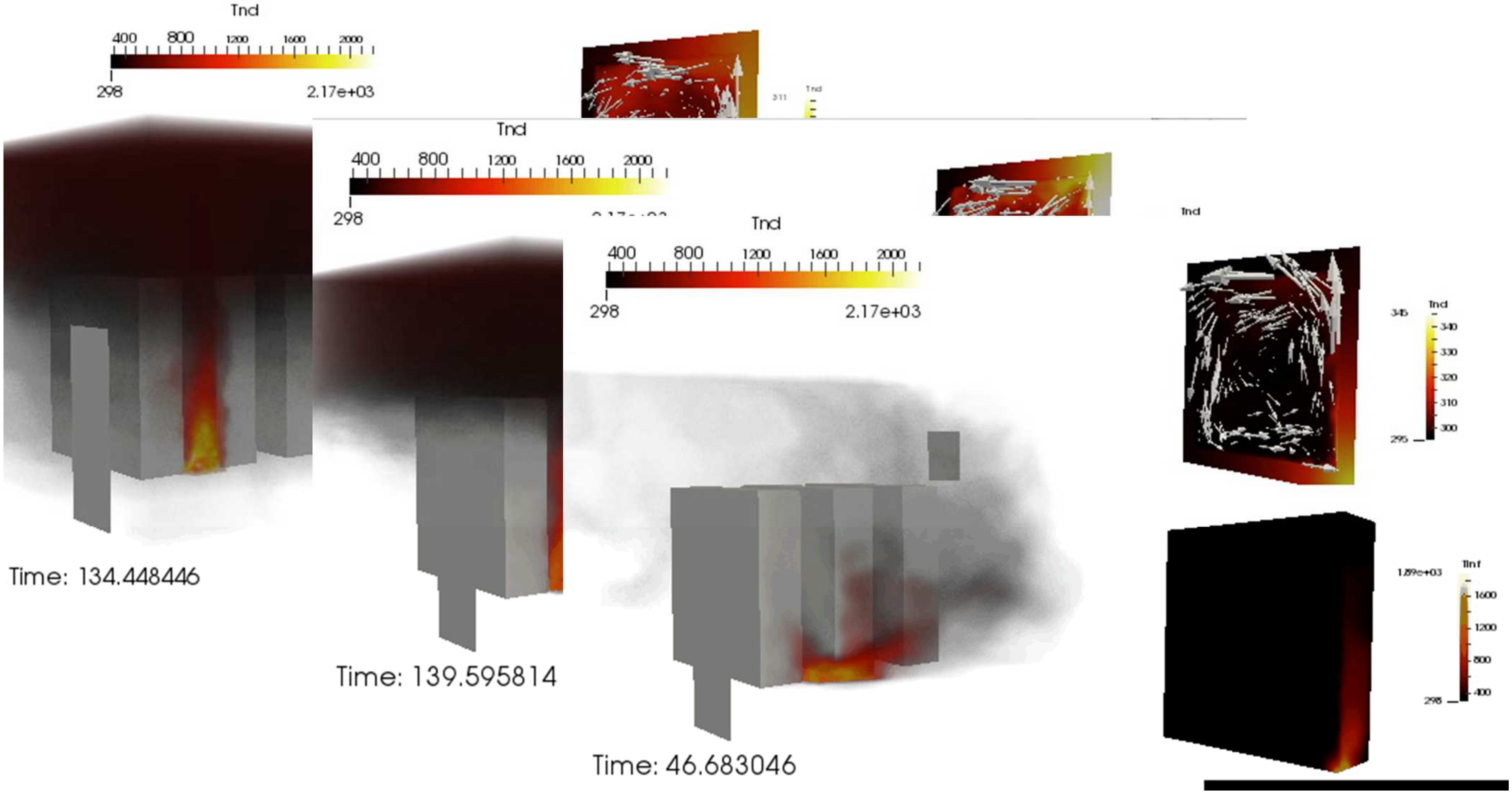
Ventilation effect on fire plume dynamics (3/3)





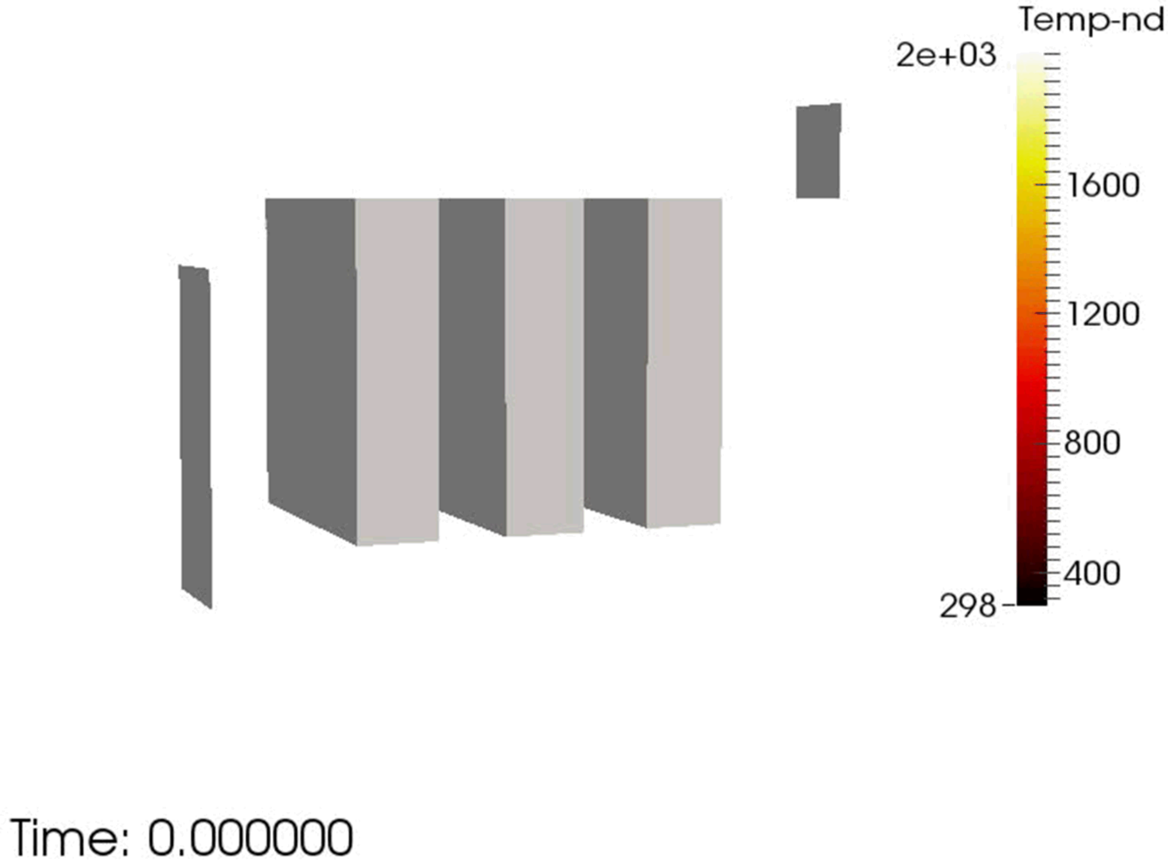
Ventilation is 10 m/s

UQ: plume dynamics



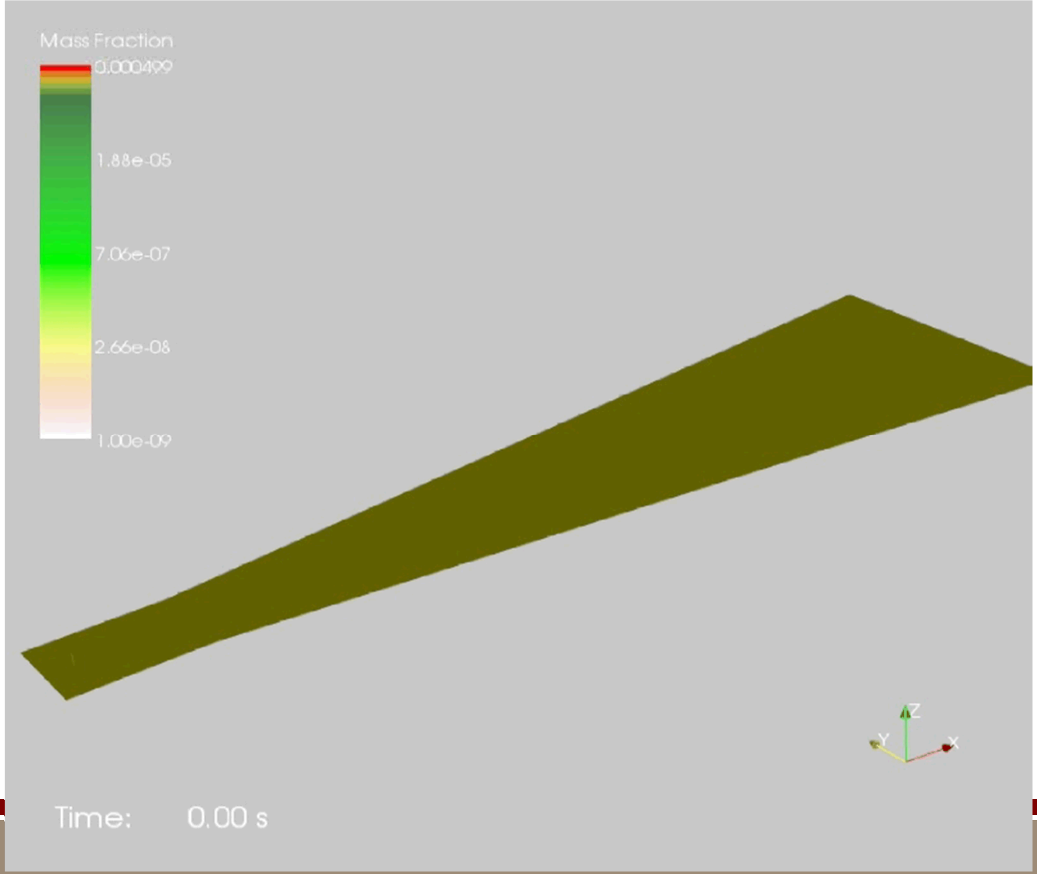
Three ventilation comparison still shot

Suppression of fires and thermal management



1 m/s Ventilation

Plumes and Hazardous Material Mapping – Concentrations as a function of time, distance, prevailing wind conditions



- Battery fire products include a range of hazardous materials:
  - HF, H_2SO_4, metals like Pb.

Summary

- Thermal runaway is a significant risk and barrier to consumer acceptance.
- Challenge: Battery technology moves forward with advances in material science.
- Modeling fire environments with conjugate heat transfer
  - Fire modeling of fuels, reactive metals, organic materials, etc. Also passivation layers, reaction within pressurizing vessels, etc.
  - Hazardous products and plume transport (HF, H_2SO_4, metals like Pb).
  - Conjugate heat transfer : mitigation through heat dissipation, chemical inhibition and active suppression.

Supporting capabilities

- UQ for accident environments.
- Sensitivity analysis to identify mitigation strategies.

THANK YOU

Questions: jchewso@sandia.gov

BACKUP MATERIAL

Sandia National Laboratories

Reactivity is heavily dependent on active materials and electrolytes (ARC results fro Pete Roth)