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PREDICTING THERMAL RUNAWAY VENT GASES: ADDRESSING FLAMMABILITY AND EXPLOSION RISKS

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PROJECT PROFILE

Topic/Vertical: Safety & Reliability

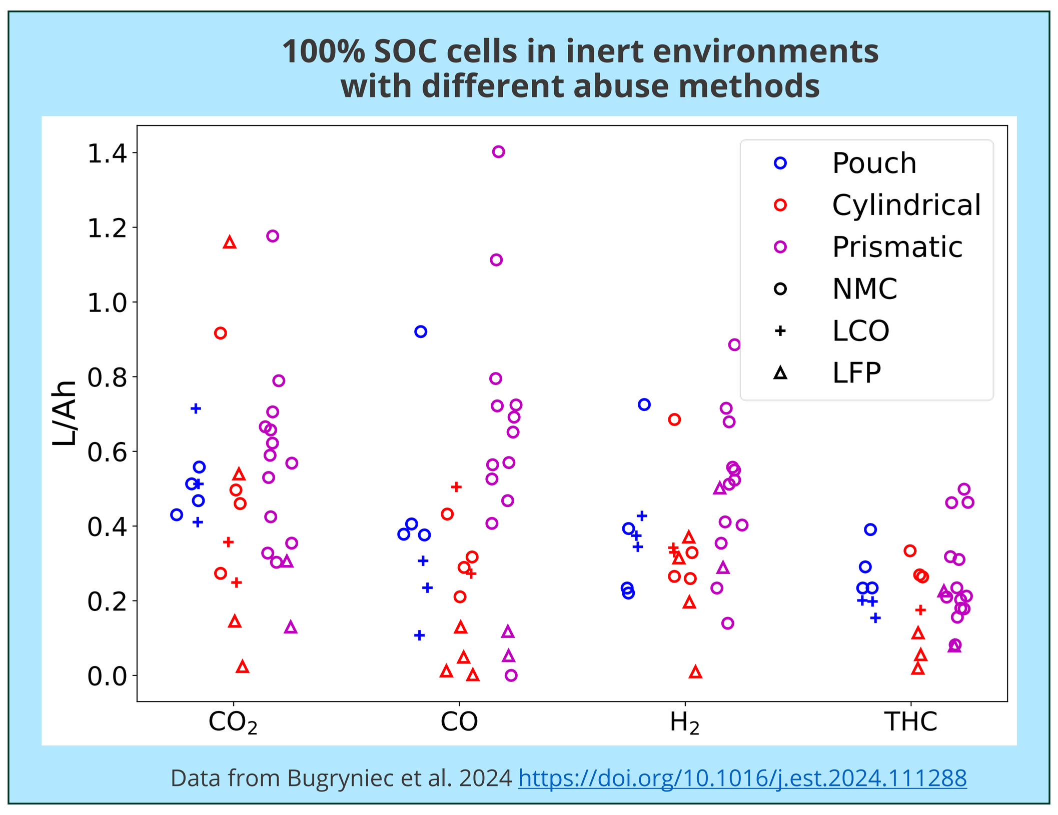
Strategic Pathway: **Stabilize:** Addressing urgent needs to ensure safety, reliability, and system security

Project start and finish: FY25-FY26

PROBLEM

Li-ion batteries in thermal runaway produce hot flammable gases that present explosion hazards and can spread fires.

- No predictive models exist for the vent gas composition. Here we tie it to Sandia-developed material-specific thermal runaway models [1].
- ***Wide flammability limits of H_2/CO/Hydrocarbon mixtures present serious risk to first responders.***
- Current practice is to measure vent gases, but wide scatter makes it difficult to identify trends.



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

APPROACH

Sandia-developed thermal runaway models are applied to cathode-electrolyte reactions that produce majority of H_2/CO.

Base cathode-electrolyte reaction [1,2]:

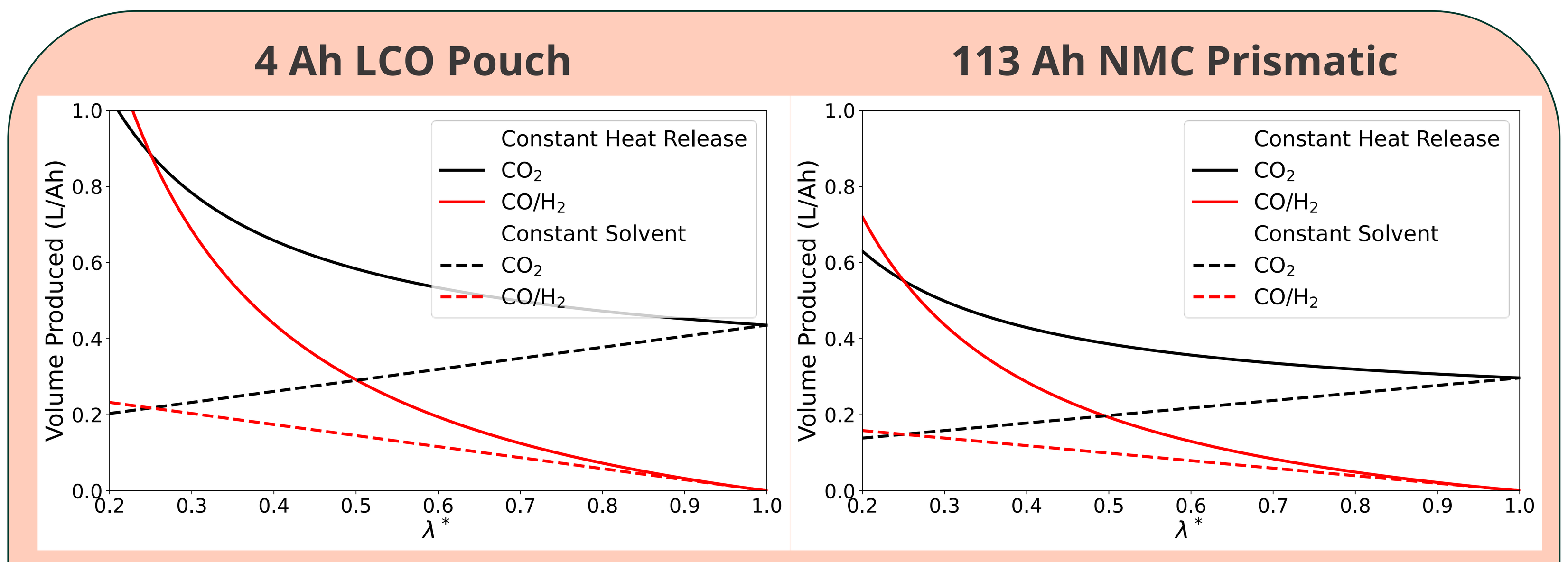
$$5MO_2 + x(CH_2O)_2CO \rightarrow 5MO + aCO_2 + bCO + cH_2O + dH_2$$

- Partial oxidation, water-gas shift reaction and electrolyte-dependent yields are used to link specific material decompositions to specific gas yields.
- Partial oxidation: $(4\lambda^* + 1)MO_2 + (CH_2O)_2CO \rightarrow (4\lambda^* + 1)MO + (2\lambda^* + 1)CO_2 + 2(1-\lambda^*)CO + 2\lambda^* H_2O + 2(1-\lambda^*)H_2$
- Water-gas shift: $CO + H_2O \rightleftharpoons CO_2 + H_2$ with $K_p = \frac{ad}{bc}$
- Two parameters: λ^*: partial-oxidation progress; K_p: equilibrium constant.

FUTURE DIRECTIONS

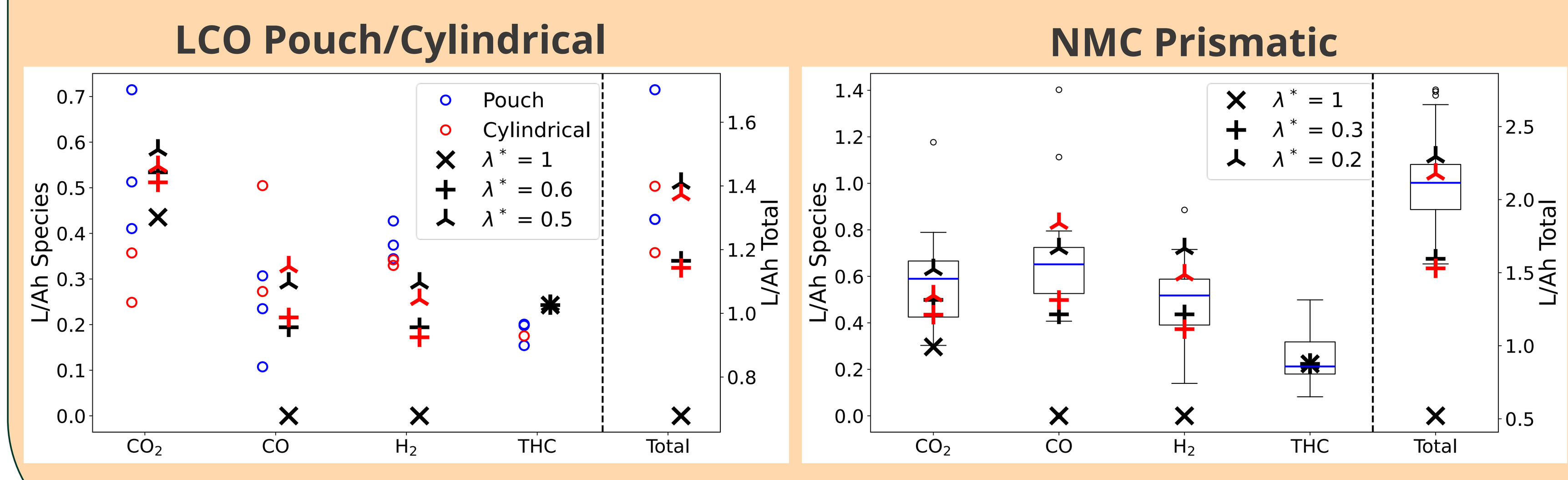
- Further analysis of anode decomposition, minor components (PVDF, carbon binder, etc.)
- Modeling of solid particles ejected with the vent gases
- Generalization to chemistries beyond Li-ion

RESULTS



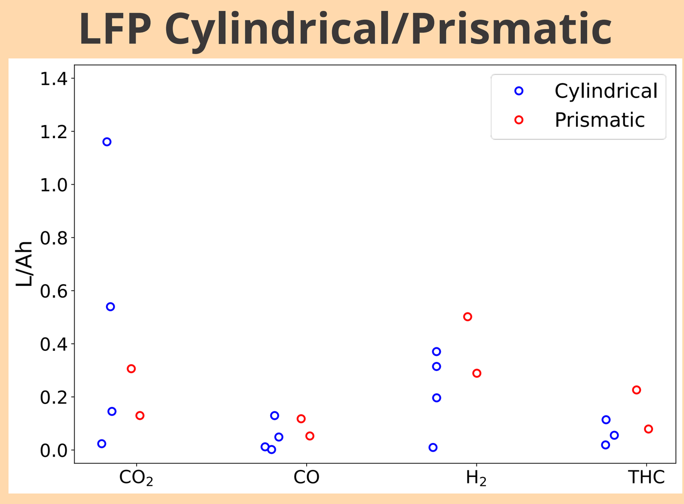
Partial oxidation releases much less heat: Unknown is fraction of electrolyte vented before thermal runaway. To get proper behavior, need more post-TR electrolyte for partial oxidation.

Partial oxidation (alone) improves gas composition prediction for layered metal oxides (black symbols). Adding water-gas partial equilibrium (red symbols) further improves CO/H2 ratio.

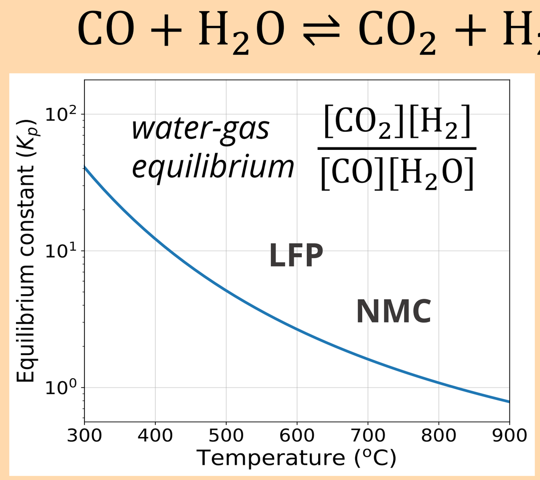


Previous full oxidation (x-symbol) misses CO and H_2.

For LFP cells, cathode chemistry doesn't explain measurements. Anode-electrolyte reaction plus water-gas shift together with lower temperatures predicts large H_2/CO ratio.



$CO + H_2O \rightleftharpoons CO_2 + H_2$



Lower temperatures for LFP with water-gas equilibrium favor observed H_2/CO ratio

CONCLUSIONS & IMPACT

Prediction of gas-compositions together with previous propagation predictions provides a materials-science based mechanism to estimate flammable gas generation rates in various large-scale thermal runaway scenarios [3].

- Partial oxidation informs the flammable (H_2 and CO) versus inert (CO_2) content. Water gas improves the H_2/CO ratio prediction.
- Use these to assess ventilation requirements for NFPA-68/69 and understand explosive risks from thermal runaway extent.

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References

[1] Shurtz and Hewson, *J. Electrochem. Soc.*, 2020 and Shurtz et al., *J. Electrochem. Soc.*, 2018.

[2] Kurzawski et al., *Fire Safety J.*, 2023 and Kurzawski, et al., *Proc. Combust. Instit.* 2020.

[3] This work is also being presented at the International Symposium on Combustion, July 2026.