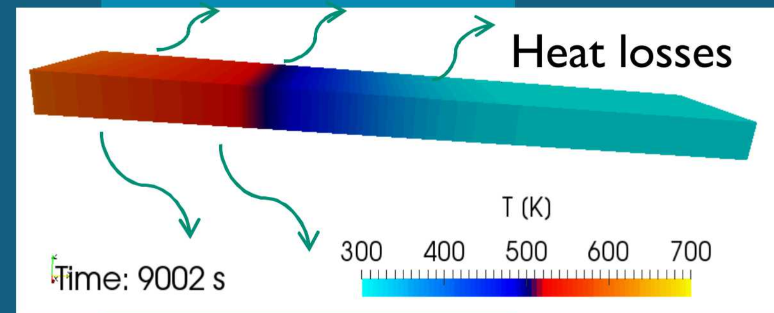
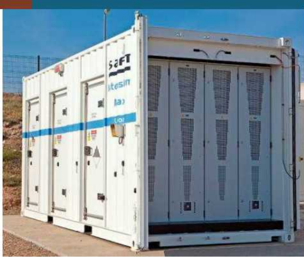
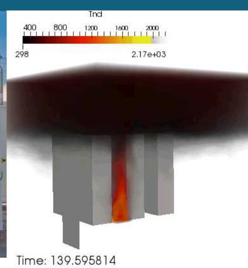
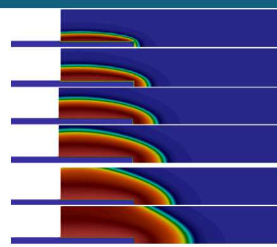
SAND2020-10619C

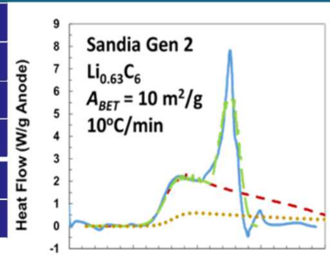
Toward predicting trends in propagating failure and its mitigation for a lithium-ion cell stack











Presented by

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Thermal runaway and cascading failure

Validated reliability and safety is one of four critical challenges identified in the Department of Energy Office of Electricity's 2013 Grid Energy Storage Strategic Plan

- Failure rates as low as 1 in several million
- Potentially many cells used in grid-scale energy storage
- Moderate likelihood of 'something' going wrong

A single point failure that propagates through the pack can have an impact even with low individual failure rates.

How do we decrease the risk?

The typical approach is to test our way into safety

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

Supplement testing with predictions of challenging scenarios and optimization of mitigation.

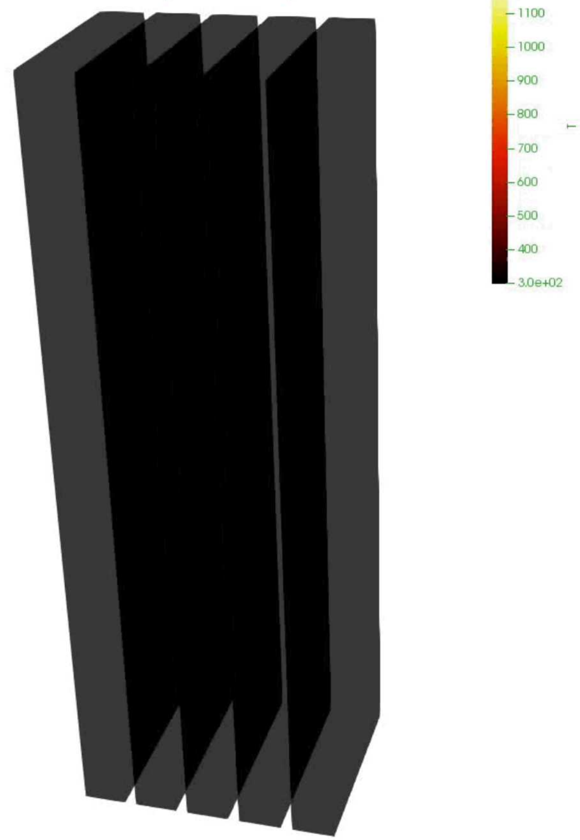
- Develop multi-physics models to predict failure mechanisms and identify mitigation.
- Build capabilities with small/medium scale measurements.
- Still requires some testing and validation.

Please excuse the lack of graphics but peripheral images removed to avoid copyright issues

Simulating cascading failure of cell stack

Short circuit simulated in first cell acts as boundary condition

Heat losses



Simulating cascading failure of cell stack

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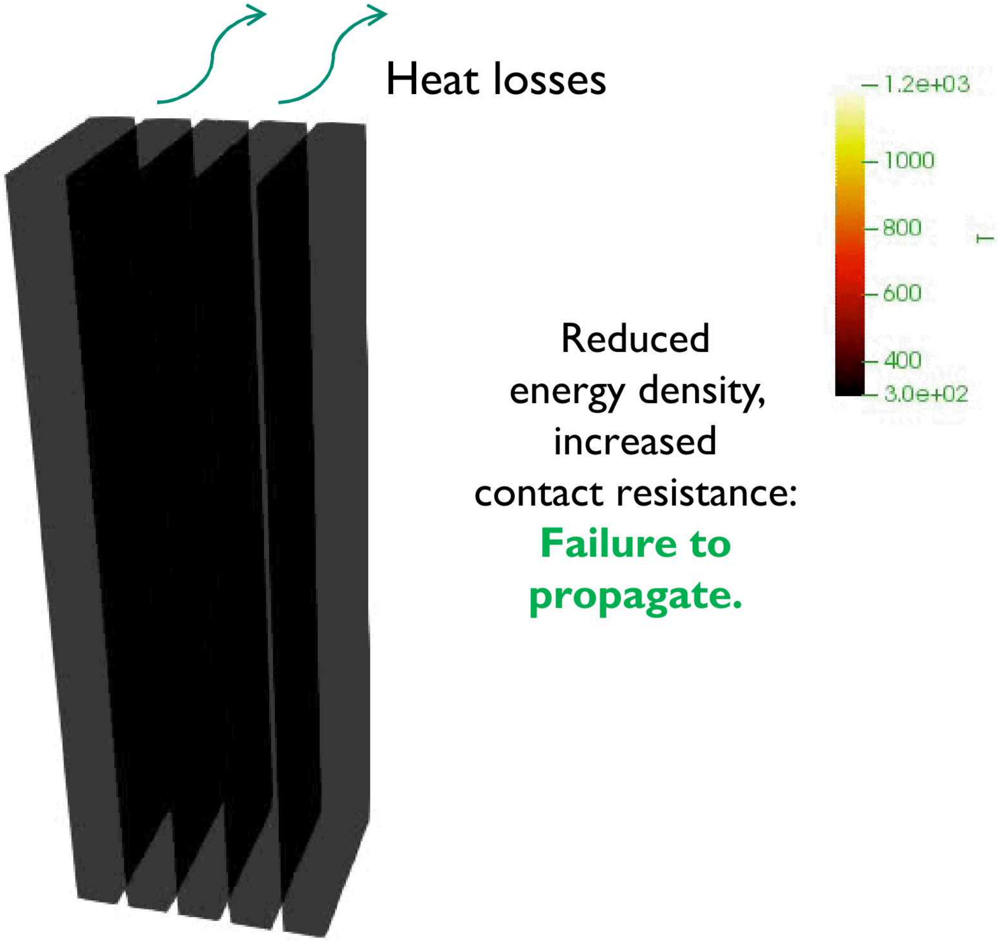


Reduced energy density, increased contact resistance: **Failure to propagate.**

Finite element model

Discretization in one direction (***x***)

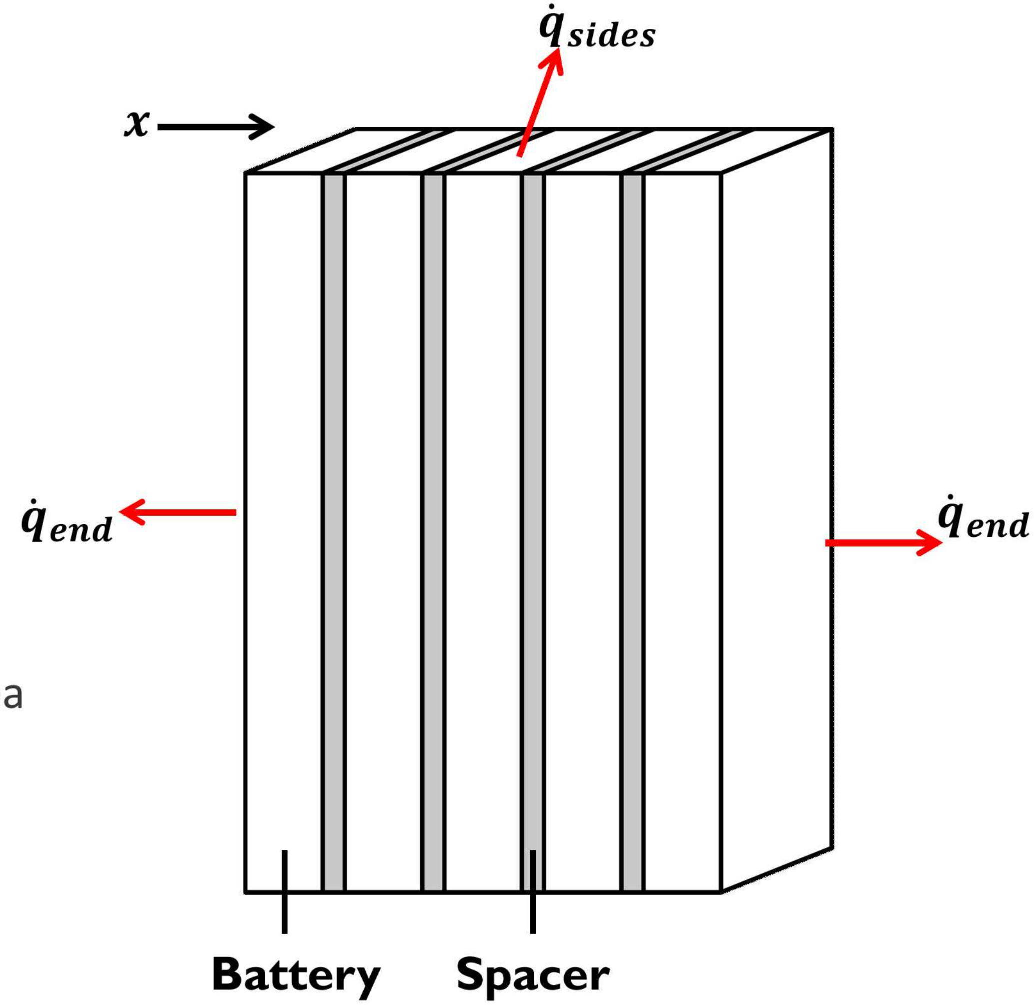
Modeled as a quasi 1-D domain of thin hexahedron elements

Multi-layered system

- Lumped battery material
- Metal plate spacers
- End block insulators
- Contact resistances between blocks/plates

Convective heat transfer to surroundings (scaled by surface area to volume ratio for thin domain)

Heat conduction with chemical sources inside battery material



Finite element model equations

Energy conservation:

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (K \nabla T) + \dot{q}'''$$

Mass conservation for species i with N_r reactions:

$$\frac{\partial \rho_i}{\partial t} = \sum_{j=1}^{N_r} (\nu''_{ij} - \nu'_{ij}) r_j$$

Energy source:

$$\dot{q}''' = \sum_{j=1}^{N_r} \Delta H_j r_j$$

Chemical source terms for thermal runaway

Empirical chemical reactions:

- SEI decomposition (Richard, et al., 1999, Shurtz, et al., 2018)

$$(CH_2OCO_2Li)_2 \rightarrow Li_2CO_3 + gas$$

- Anode-electrolyte (Richard, et al., 1999, Shurtz et al., 2018, Kurzawski et al., 2020)

$$2C_6Li + C_3H_4O_3 \rightarrow 2C_6 + Li_2CO_3 + gas$$

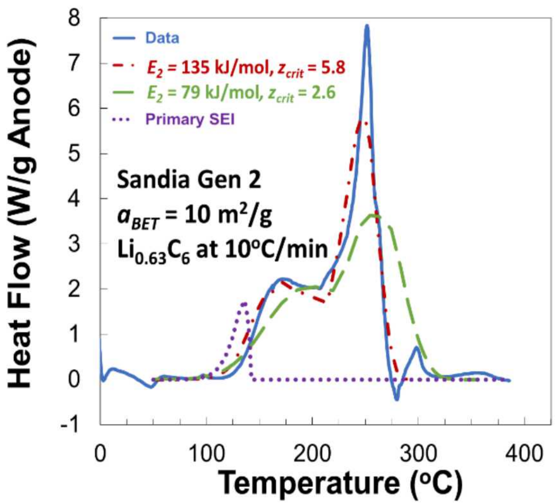
- Cathode-electrolyte (Hatchard, et al. 2001, Shurtz, et al., 2020, Kurzawski et al., 2020)

$$CoO_2 + \frac{2}{15}C_3H_4O_3 \rightarrow \frac{1}{3}CoO + gas$$

- Short-circuit (Kurzawski, et al., 2020)

$$C_6Li + CoO_2 \rightarrow C_6 + LiCoO_2$$

2018 anode models



References for kinetics models

- Shurtz, et al., *J. Electrochem. Soc.*, 165, A3878 (2018).
- Shurtz, et al., *J. Electrochem. Soc.*, 165, A3891 (2018).
- Richard and Dahn, *J. Electrochem. Soc.*, 146, 2078 (1999).
- Hatchard, et al., , *J. Electrochem. Soc.*, 148, A755 (2001).
- Shurtz and Hewson, *J. Electrochem. Soc.*, 167, 090543 (2020)
- Kurzawski, et al., *Proc. Combust. Instit.*, 34 (in press 2020)

Cascading failure testing

$LiCoO_2$ 3Ah pouch cells

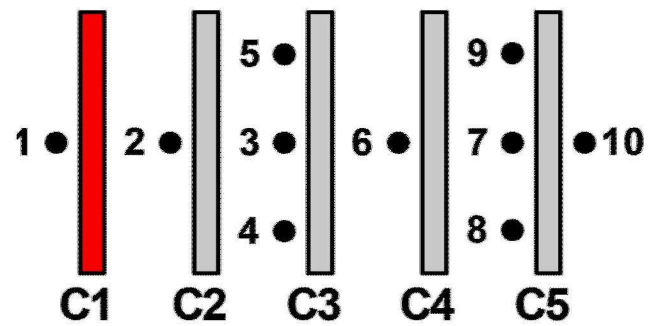
5 closely packed cells with/without aluminum or copper spacer plates

- Spacer thicknesses between 1/32” and 1/8”
- State of charge between 50% and 100%

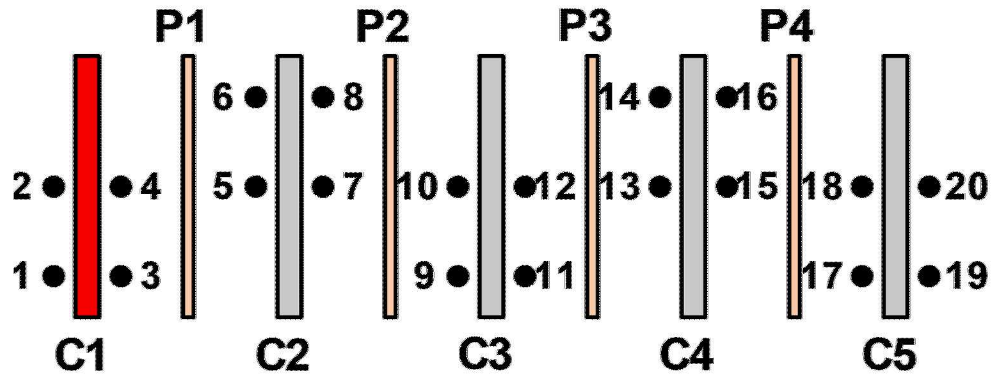
Failure initiated by a mechanical nail penetration in the outer cell (cell 1)

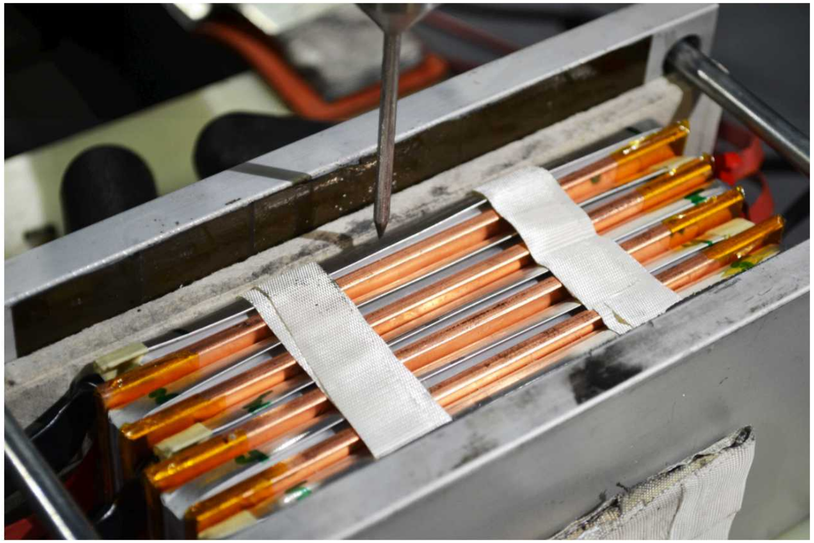
Thermocouples (TC) between cells and spacers (if present)

Thermocouple Locations



Thermocouple Locations with spacer plates

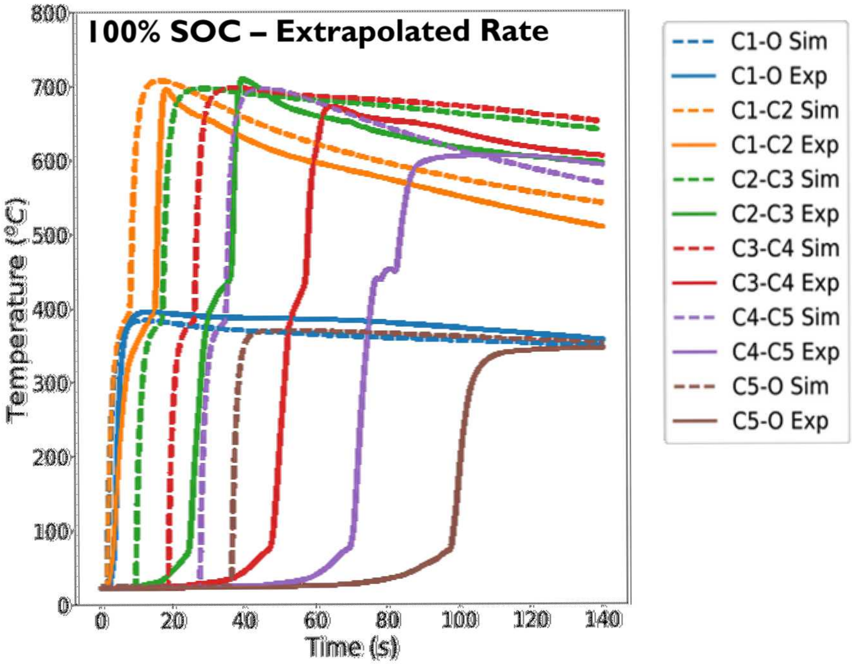




Torres-Castro, L. et al., (2020) J Electrochem. Soc., **167**(9): 090515
Lamb, J., et al. (2015). J. Power Sources **283**: 517-523.

Predictions extrapolating early thermal runaway models to full heat release

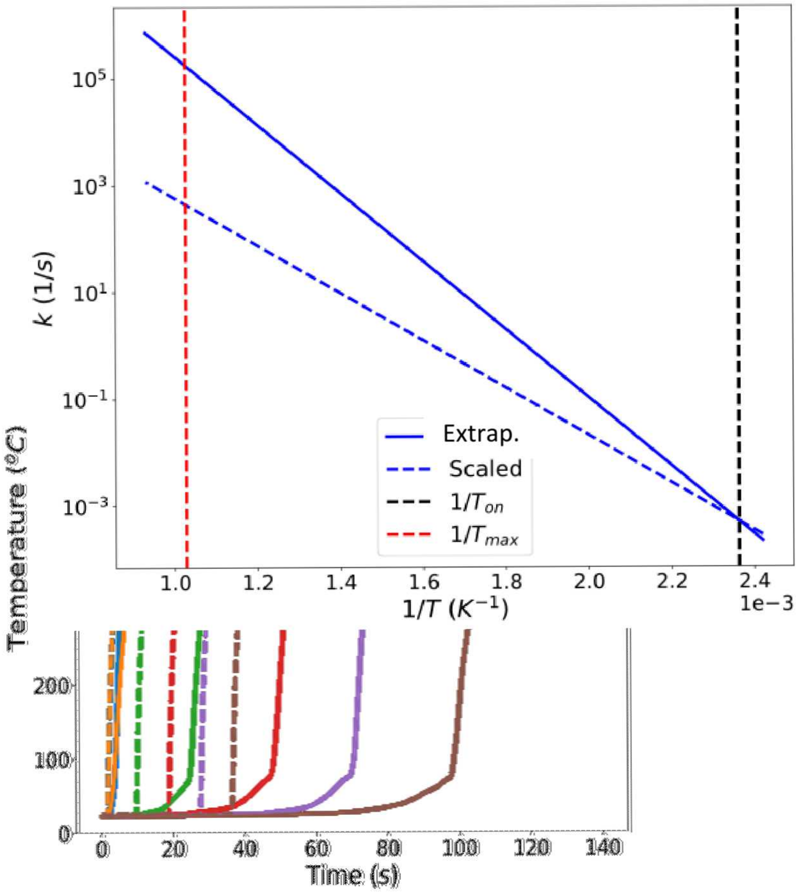
Extrapolating rate constants with full thermodynamic heat release leads to propagation predictions that are far too fast.



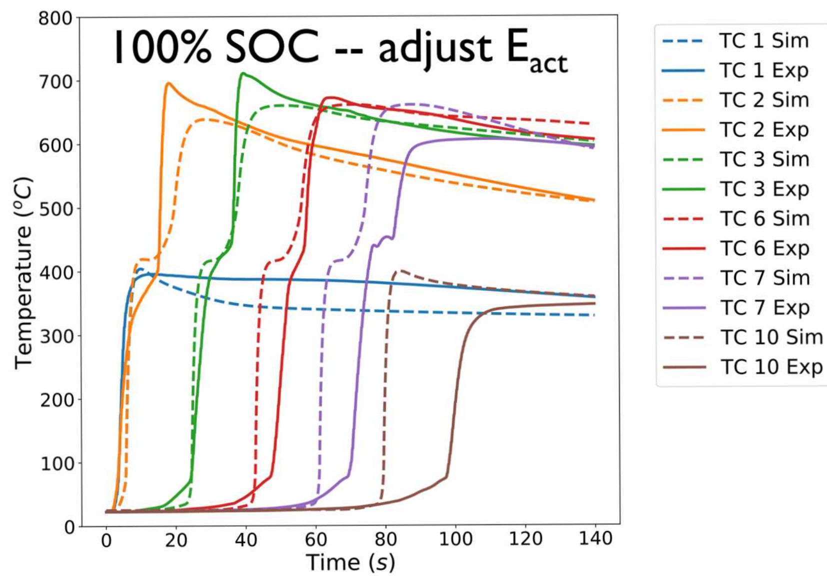
- Predictions use rate constants from
  - Anode-electrolyte: Shurtz, et al., 2018 (activation energy like Richards et al., 1999)
  - Cathode-electrolyte : Hatchard, et al., 2001 with heat of reaction following Shurtz et al., 2020
- Heat release is determined here from thermodynamics of complete reaction as reviewed in cited papers.

Propagation speed for reacting fronts scale with reaction rate at peak temps and thermal diffusivity: $v \approx \sqrt{\dot{\omega}\alpha}$

Adjusting activation energies to limit high temp rates

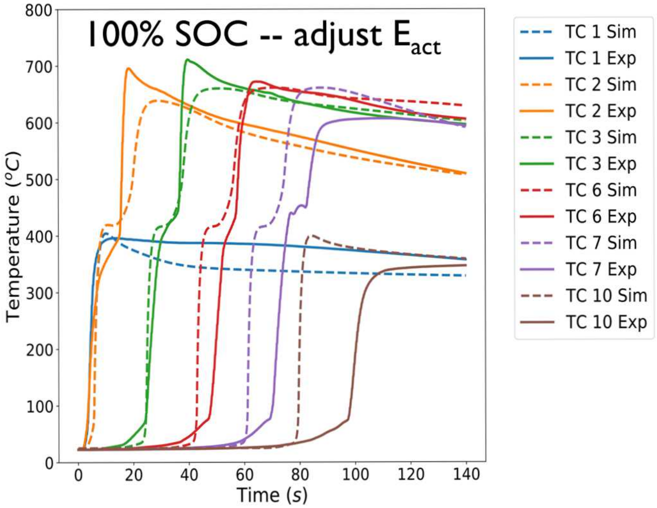


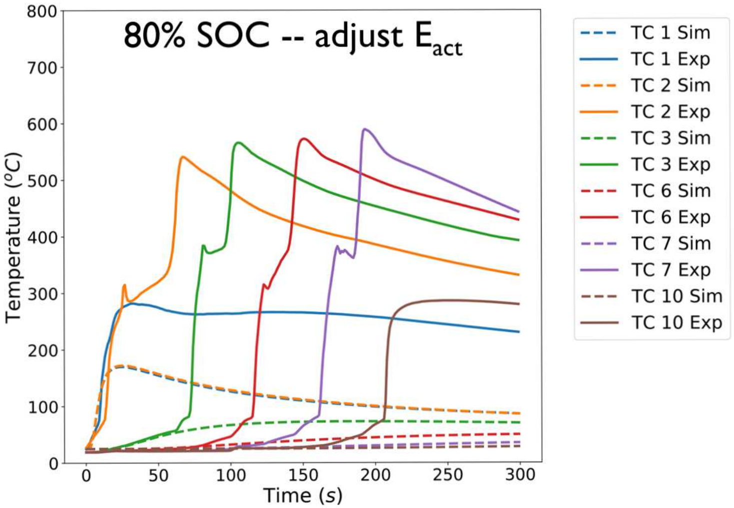
We limit high temperature rates while fixing the onset rate by adjusting the Arrhenius pre-exponential and activation energy together.

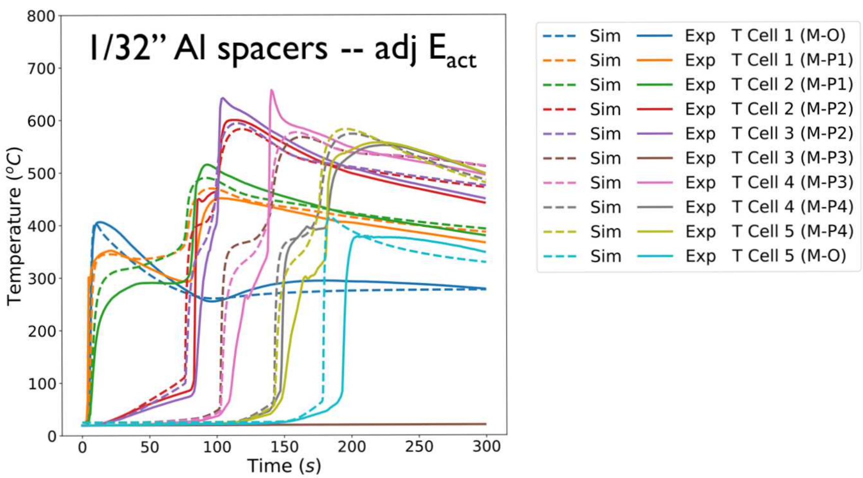


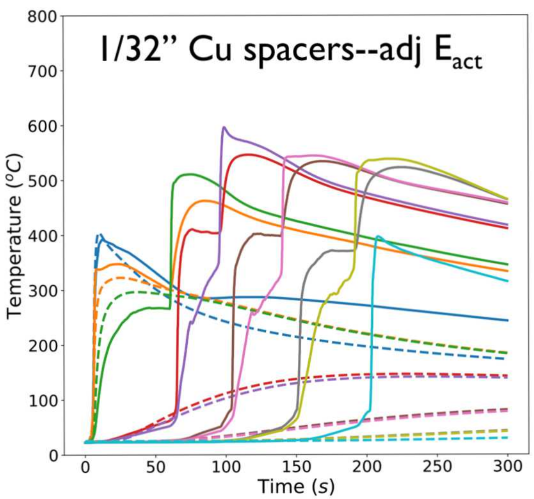
Propagation speed for reacting fronts scale with reaction rate at peak temps and thermal diffusivity: $v \approx \sqrt{\dot{\omega}\alpha}$

Adjusted activation energy looks good at 100% SOC, but does not predict full range: 100% SOC, no spacers









Adjusted activation energy predicts mitigation too soon. Lacks physical basis.

Solid-state particle diffusion can be limiting in Li-ion cells. Incorporate internal diffusion limits in series with kinetics.

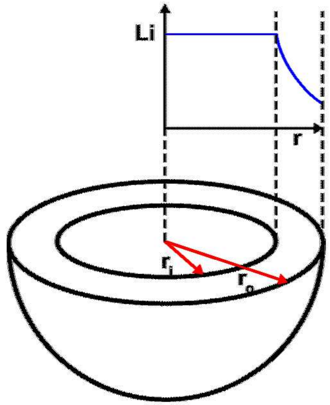
Challenge: Calorimetry measurements only at lower temperatures.

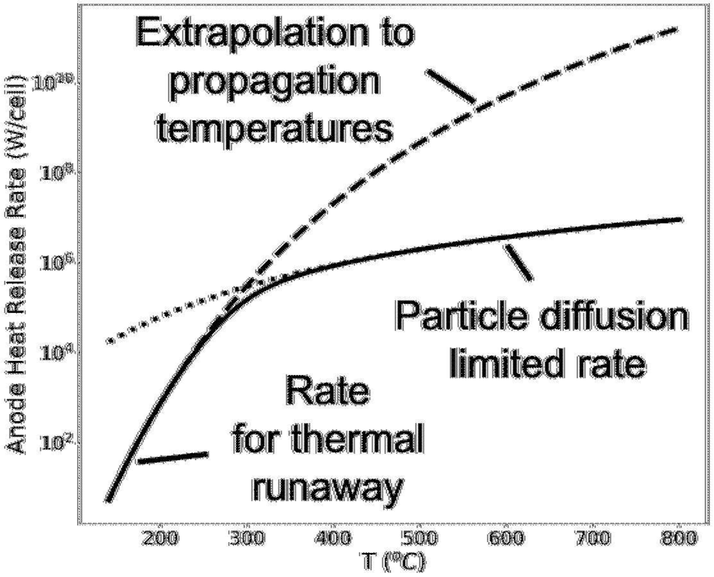
- Lithium and oxygen must diffuse to the particle surface to react with the electrolyte.
- Serial reactions are corrected with the "Damköhler limited" form.

$$k' = \frac{k}{1 + Da}$$

- Damköhler number is ratio of surface reaction rate to the rate of diffusion between an inner radius (r_i) and outer radius (r_o).

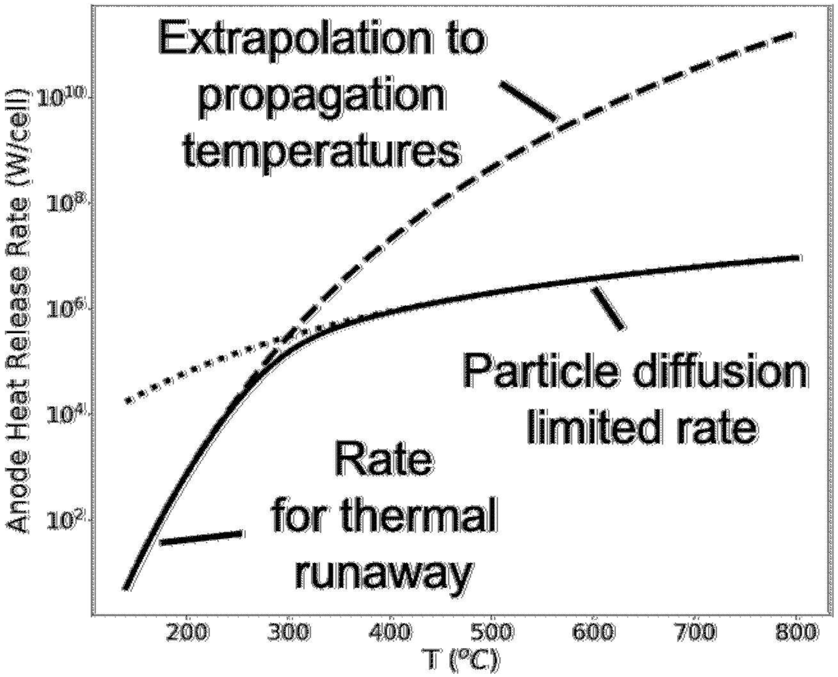
$$Da = \frac{A exp\left(-\frac{E}{RT}\right)}{a_e \rho D_o \exp\left(-\frac{E_D}{RT}\right)} \frac{(r_o - r_i)r_o}{r_i}$$

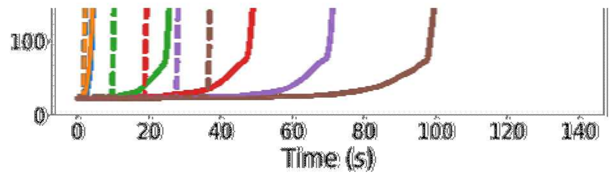




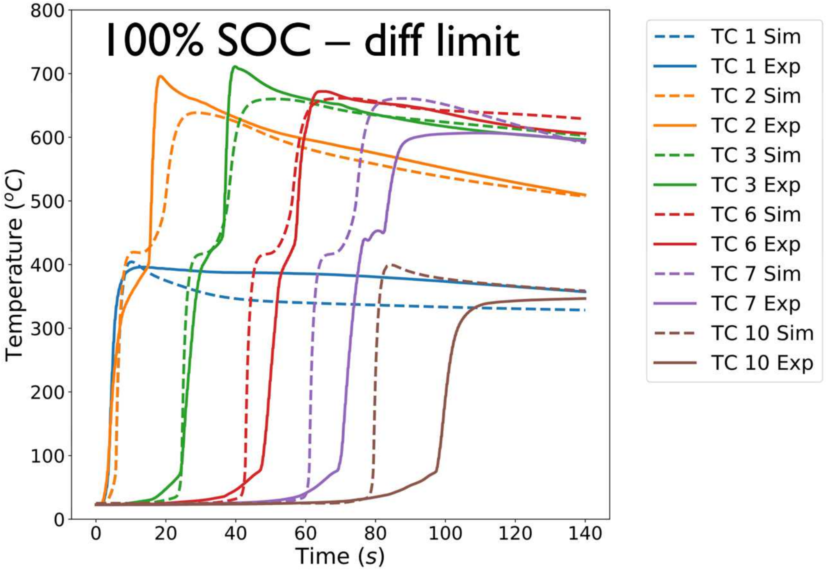
Kurzawski, A., et al. (in press 2020). "Predicting cell-to-cell failure propagation and limits of propagation in lithium-ion cell stacks." Proc. Combust. Instit. **38**.

Rate limitation at high temperature assuming transition to solid-state diffusion limited regime





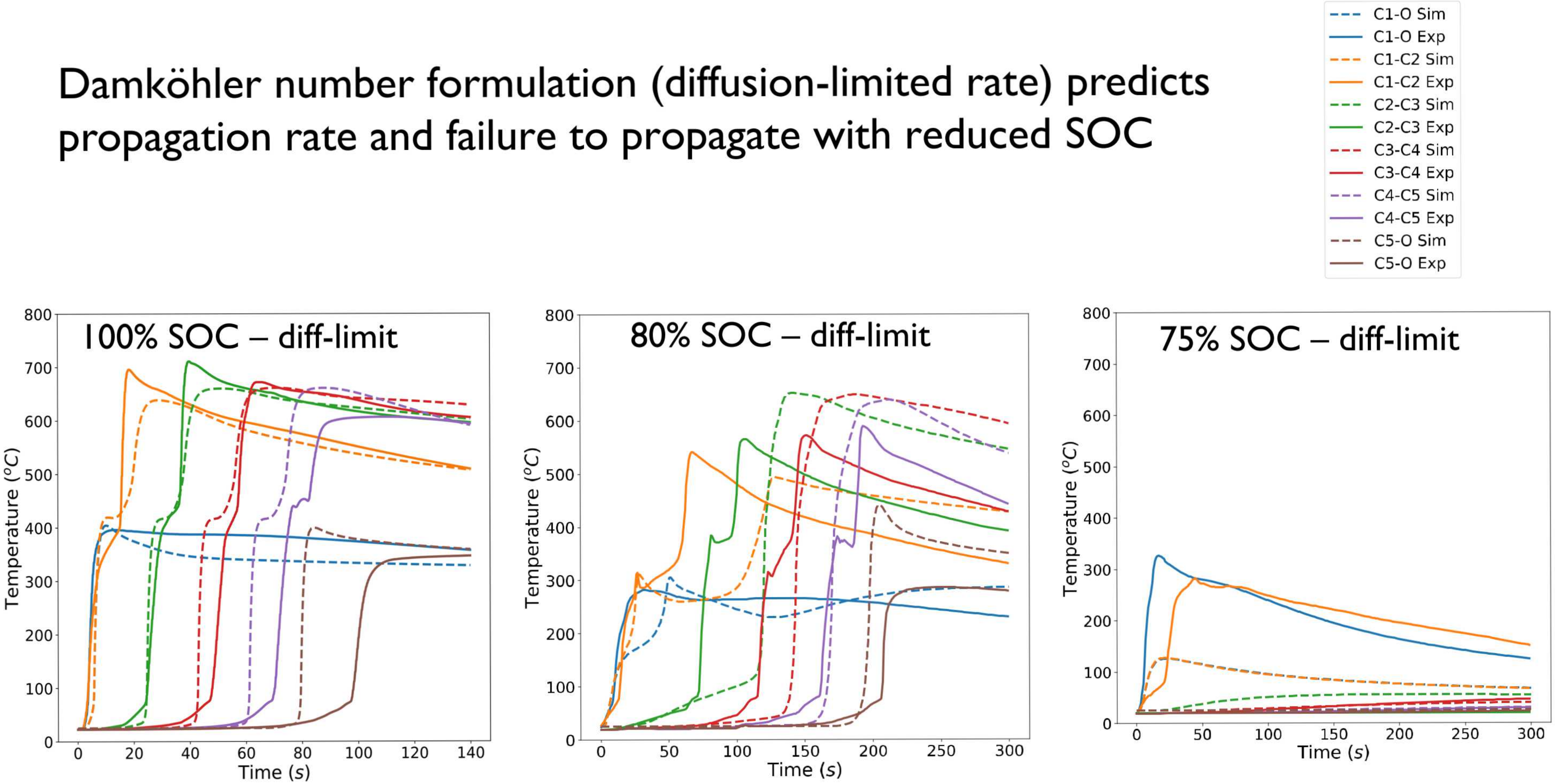
Damköhler number formulation adjusts propagation rate to reasonable degree based on literature diffusion rates



Propagation speed for reacting fronts scale with reaction rate at peak temps and thermal diffusivity: $v \approx \sqrt{\dot{\omega}\alpha}$

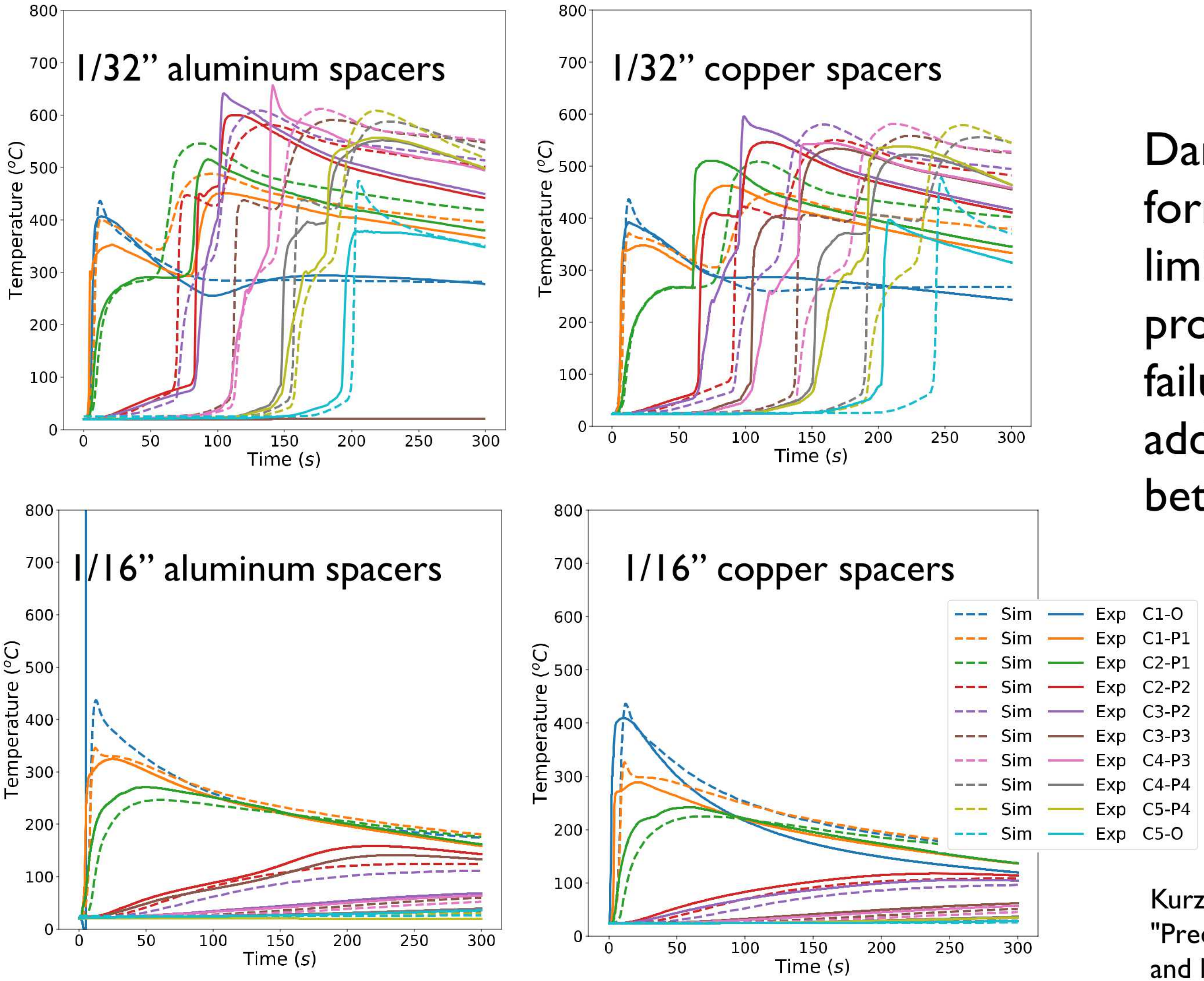
Propagation trends well-predicted with transition to solid-state diffusion limited regime

Damköhler number formulation (diffusion-limited rate) predicts propagation rate and failure to propagate with reduced SOC



Kurzawski, A., et al. (accepted 2020). "Predicting cell-to-cell failure propagation and limits of propagation in lithium-ion cell stacks." Proc. Combust. Instit. **38**.

Diffusion-limited rate predictions extend to capture effects of added metal plates between cells



Damköhler number formulation (diffusion-limited rate) predicts propagation rate and failure to propagate with added metal plates between cells

Kurzawski, A., et al. (in press 2020). "Predicting cell-to-cell failure propagation and limits of propagation in lithium-ion cell stacks." Proc. Combust. Instit. **38**.

Summary – Predicting trends in propagating failure and its mitigation

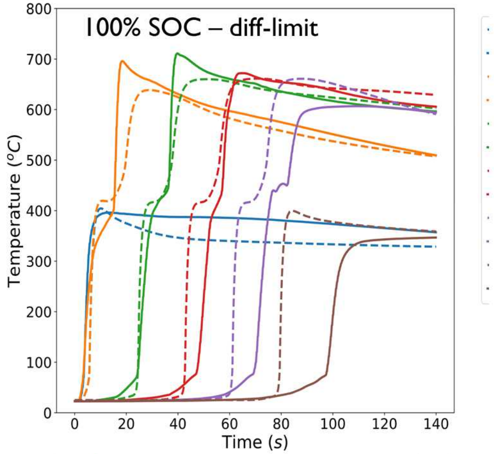
Reductions of specific energy have been measured to slow and mitigate propagation (SOC, metal plates).

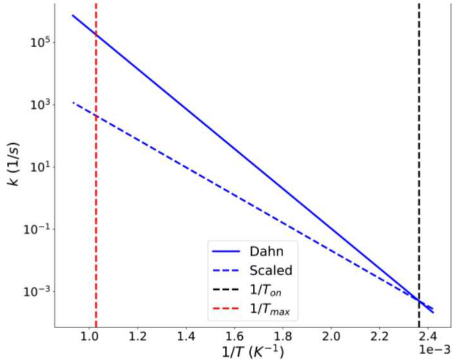
Using early source term models with 'thermodynamics' heat release leads to too fast propagation.

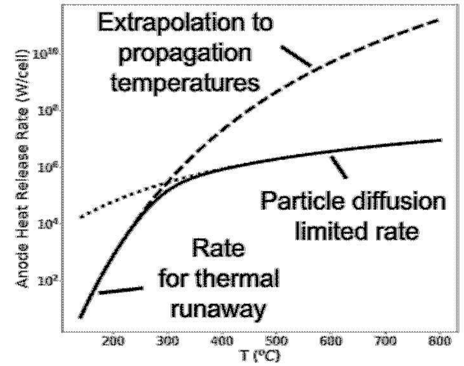
Simply adjusting activation energy matches some thermal runaway conditions but predicts mitigation too soon.

Introducing a diffusion-limit in series with kinetics predicts full range of propagation/mitigation measured recently.

Early diffusion-limit model in Kurzawski et al., 2020 to be supplemented with forthcoming publication.







Contact

Thank you

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