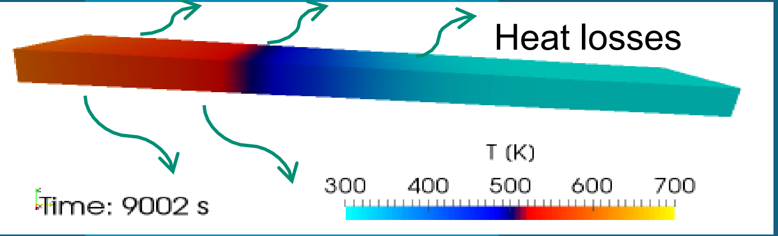
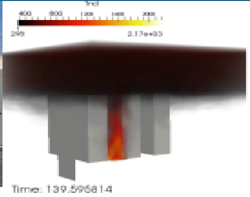
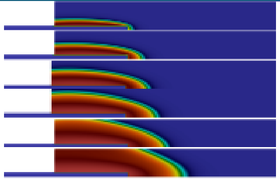
SAND2021-12877C

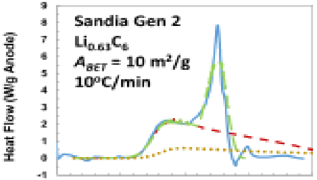
Sandia National Laboratories

LIM1TR: Lithium-ion Modeling with 1-D Thermal Runaway









Presented by

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Department of Energy Office of Electricity

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Thermal runaway and cascading failure

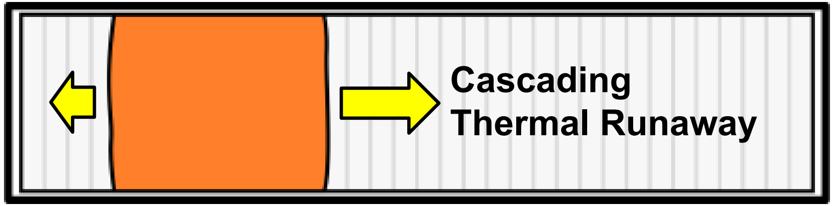
Cascading failure poses a risk to ESS installations and first responders.

The current approach is to test our way into safety

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

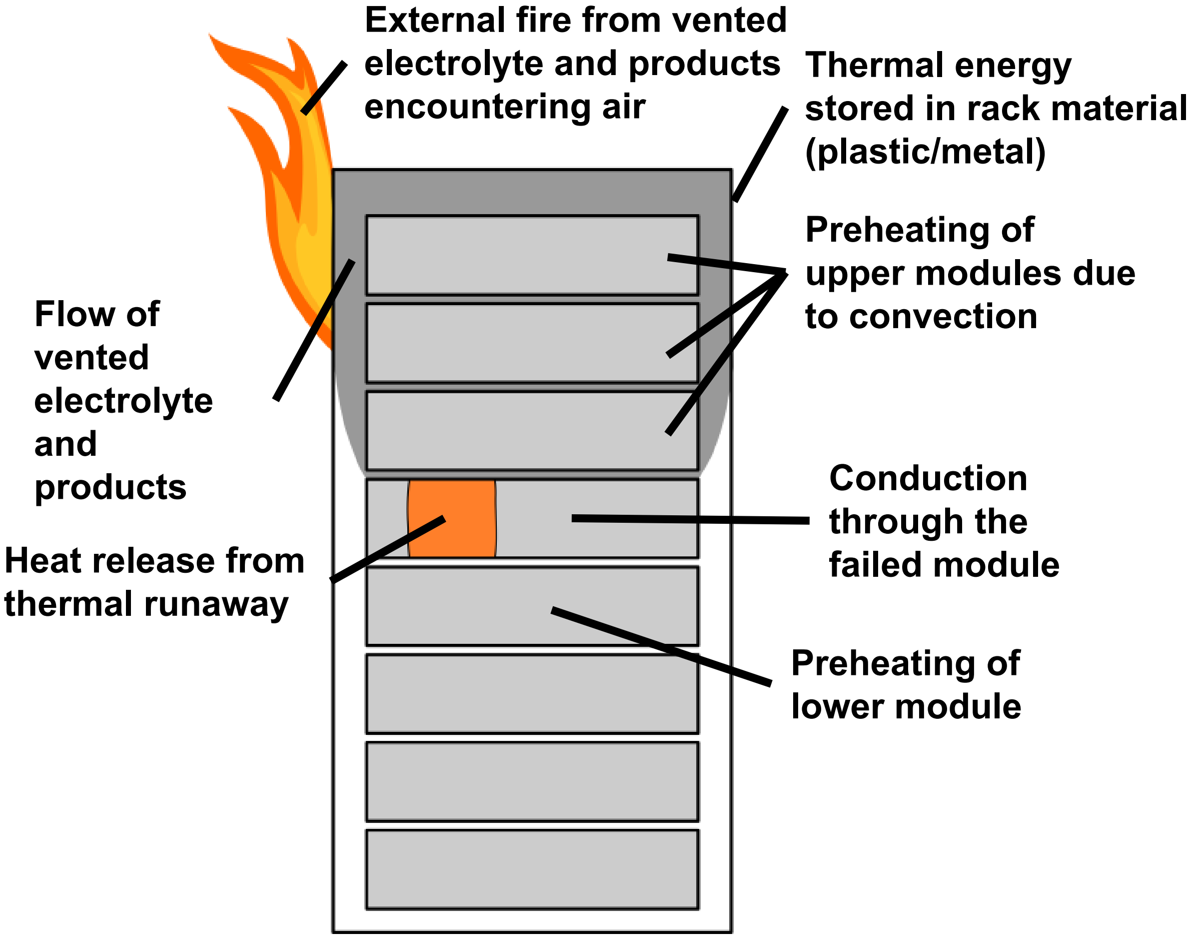
Supplement testing with predictions of challenging scenarios and optimization of mitigation.

A key to designing safe systems at larger scales is understanding cascading thermal runaway.



Source: (top) https://cmte.ieee.org/pes-essb/wp-content/uploads/sites/43/2019/06/2019-SM-UL-9540A-IEC-Lithium-Test-Sumr
(bottom) https://www.lgessbattery.com/eu/grid/product-info.lg

Energy flows at the rack/system scale

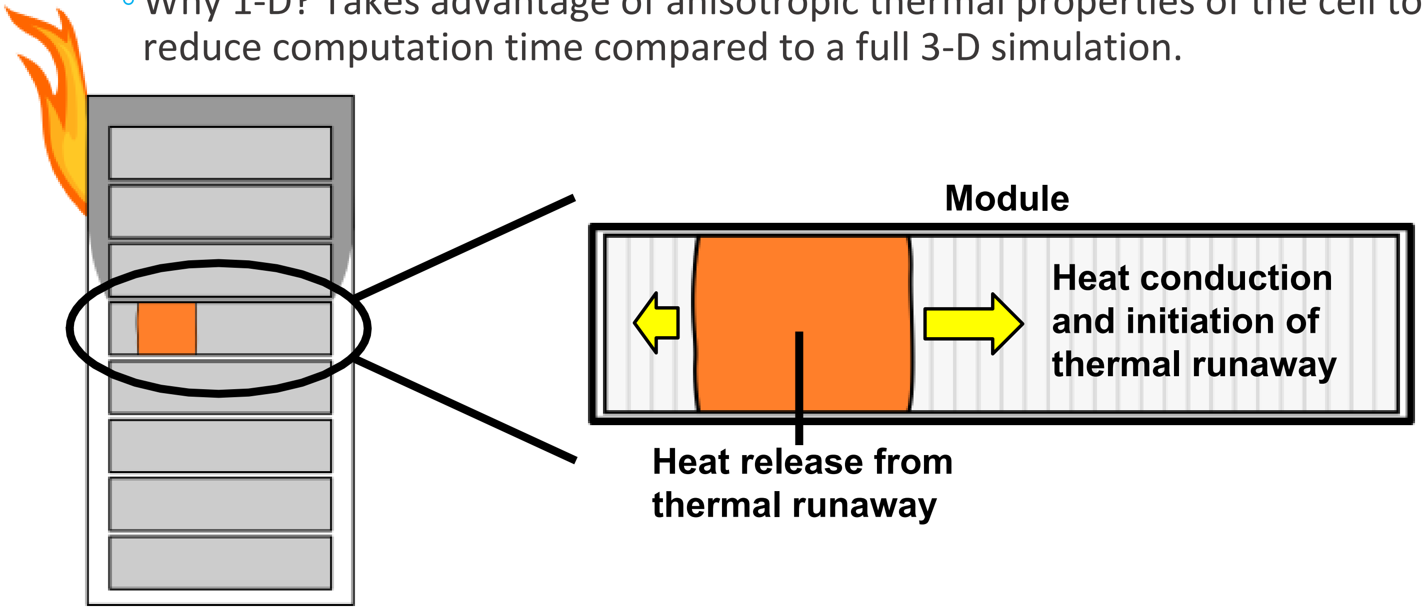


Objective: simulate energy flows at the module scale

Examining the energy flows in an ESS, cascading failure at the module level is the primary source of energy (produces flaming gases, ignites plastics).

The **LIM1TR** (Lithium-ion Modeling with 1-D Thermal Runaway) software simulates the cascading thermal runaway problem at the module level.

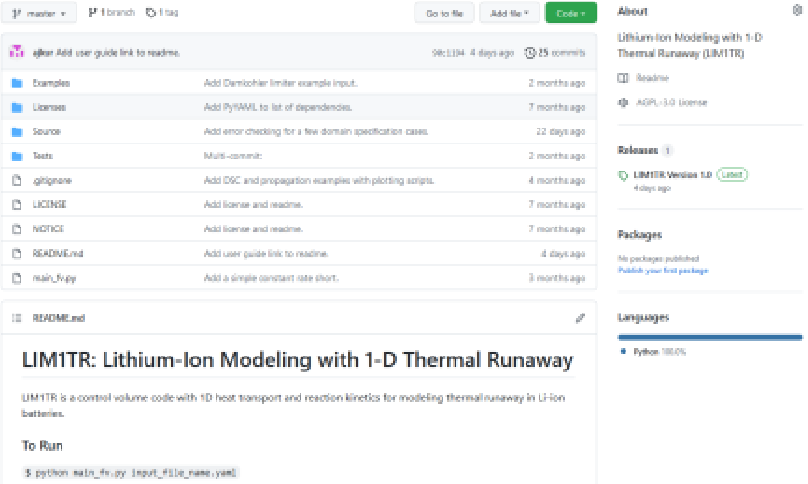
- Why 1-D? Takes advantage of anisotropic thermal properties of the cell to greatly reduce computation time compared to a full 3-D simulation.

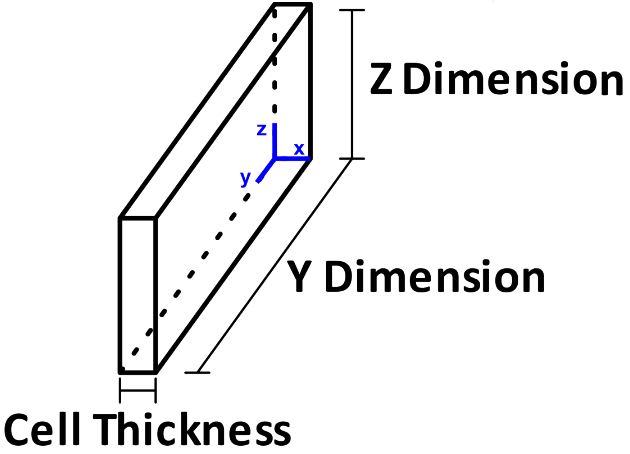


Overview of **LIM1TR**

Features
- Open source software:
  - https://github.com/ajkur/lim1tr
  - Compatible with Linux and Windows
- Written in Python with plain-text 'yaml' user input
- A set of unit and verification tests checks the code's operation and numerics
- Flexible user-specified chemistry inputs
- User Guide: SAND2021-12281

Solution methodology:
- Quasi 1-D finite volume model thermally lumped in the y and z dimensions (plane of electrodes)
- Discretized in the x direction
- Operator splitting for time integration

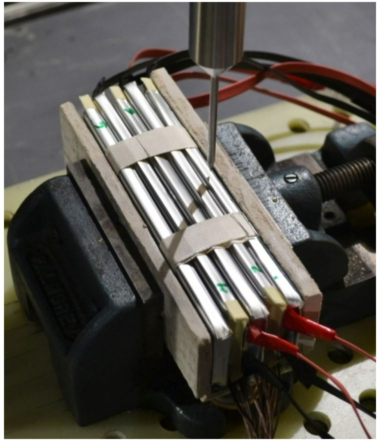




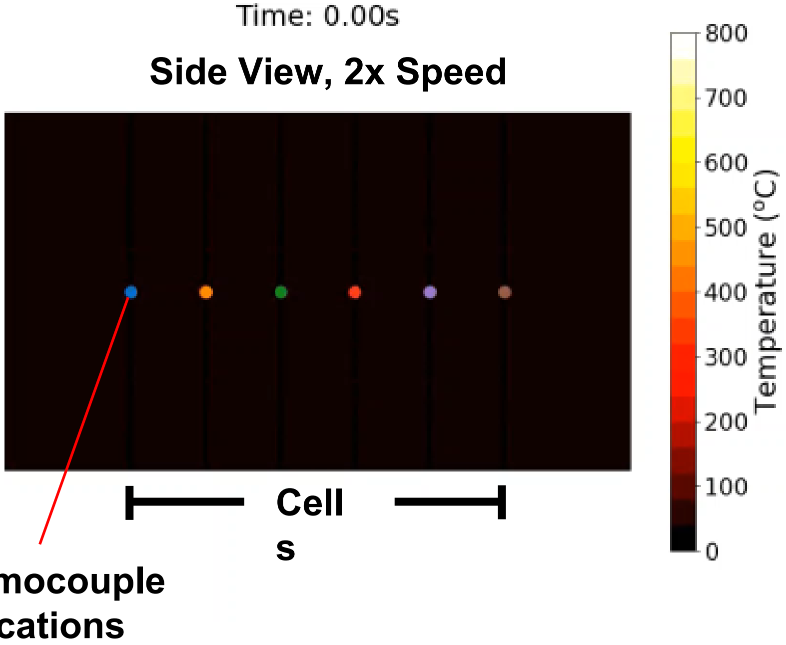
Cascading failure predictions at the module scale: 5 cell stack

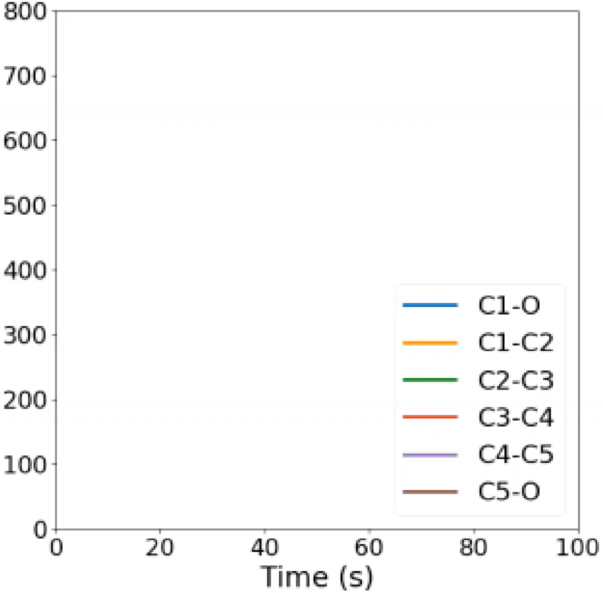
Nail penetration test in a stack of 5 lithium cobalt oxide pouch cells (3Ah).
- Experiments from Torres-Castro et al. 2020.

Top Perspective View



Side View, 2x Speed





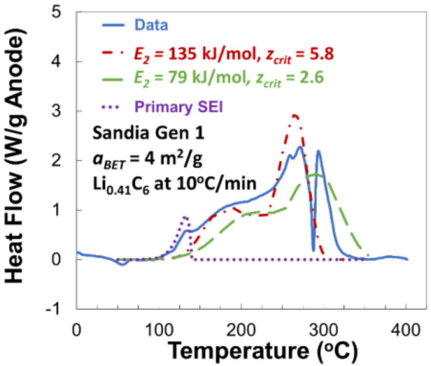
Cascading failure example simulation: input file

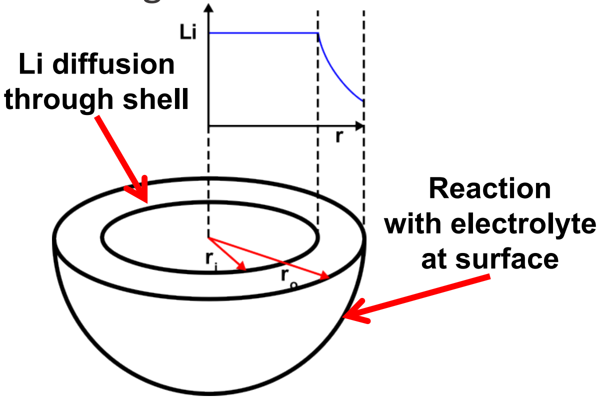
```yaml
Materials:
    Battery:
        k: 0.5
        rho: 1815.0
        cp: 770.0
    Backer:
        k: 0.36
        rho: 1356.0
        cp: 1500.0

Species:
    Names: ['EC', 'C6Li', 'SEI', 'Salt1', 'Li2CO3', 'C6', 'CoO2', 'Co3O4', 'LiCoO2', 'AllGas', 'Container']
    Initial Mass Fraction: [0.0539, 0.1329, 0.0136, 0.0, 0.0, 0.0, 0.1468, 0.0054, 0.0, 0.0015, 0.6459]
    Molecular Weights: [88.062, 79.007, 161.952, 73.89, 73.89, 72.066, 90.931, 240.795, 97.872, 1.0, 0.0]
    Material Name: Battery

Reactions:
    1:
        A: 3.707251453e+16
        E: 16236.69403
        R: 1
        H: -635000.0
        Reactants:
            'SEI': 1
        Products:
            'Salt1': 1
            'AllGas': 88.062
        Orders:
            'SEI': 0.5
    2:
        A: 3.2718e+13
        E: 135000.0
        R: 8.3145
        H: -2287100.0
        Reactants:
            'C6Li': 2
            'EC': 1
        Products:
            'C6': 2
            'Li2CO3': 1
            'AllGas': 28.054
        Type: 'Zcrit'
        BET_C6: 1.1
        tau_crit: 0.08
        C_t: 72.5
        Y_Graphite: 0.1212044831
        Electrolyte Limiter:
            Species: 'EC'
            Limiting Constant: 1.2
        Damkohler:
            D: 3.67e-14      # m2/s
            E: 35000.0       # J/mol
            A: 2.1e+13       # 1/s
            r_i: 1.0e-6      # m
            r_o: 2.0e-6      # m
```

Input file allows for specification of the materials, reactions, boundary conditions, and simulation domain.

Flexible reaction specification allows for advanced chemical models.

- Critical thickness model for the anode
- Damköhler limiter model for both electrodes
- Care must be taken in constructing reaction constants

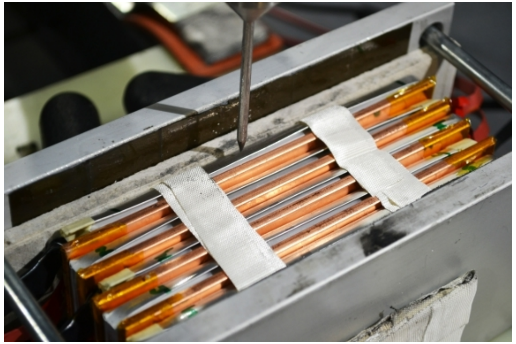




R. Shurtz, J. Engerer, J. C. Hewson, "Predicting high-temperature decomposition of lithiated graphite with electrolytes: I. Review of phenomena and a comprehensive model," *J. Electrochem. Soc.*, (December 2018).
R. Shurtz, J. Engerer, J. C. Hewson, "Predicting high-temperature decomposition of lithiated graphite with electrolytes: II. Predicting passivation layer evolution and the role of surface area," *J. Electrochem. Soc.*, (December 2018).
A. Kurzawski, L. Torres-Castro, R. Shurtz, J. Lamb, J. C. Hewson, "Predicting cell-to-cell failure propagation and limits of propagation in lithium-ion cell stacks," *Proc. of the Combustion Institute*, (January 2021).

Mitigation of cascading failure at the module scale: 5 cell stack with 1/8” copper spacers

Top Perspective View



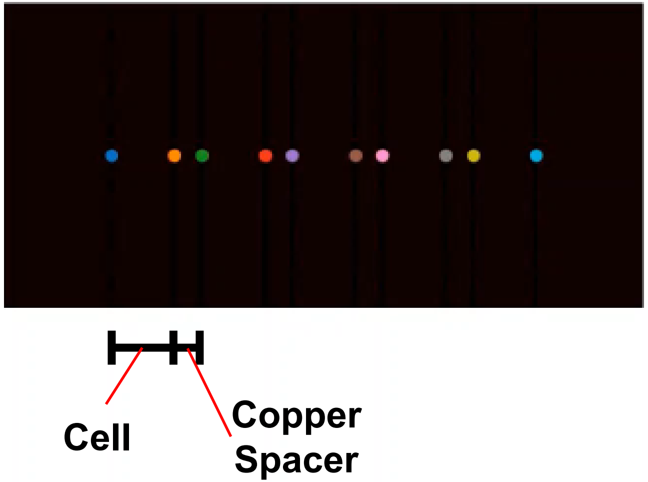
The **LIM1TR** input file can be easily modified to include more layers.

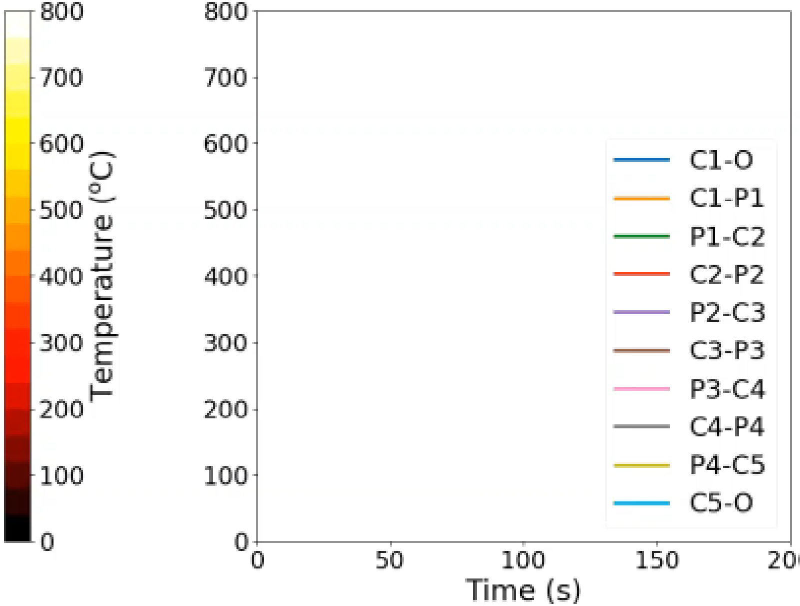
The added thermal mass of the copper mitigates cascading failure.

Propagation/mitigation is still captured despite fidelity loss in 1-D.

Time: 0.00s

Side View, 2x Speed



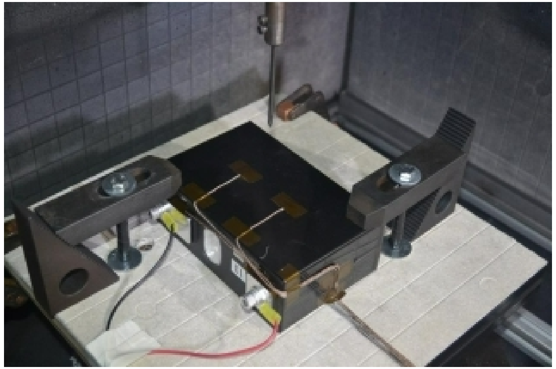


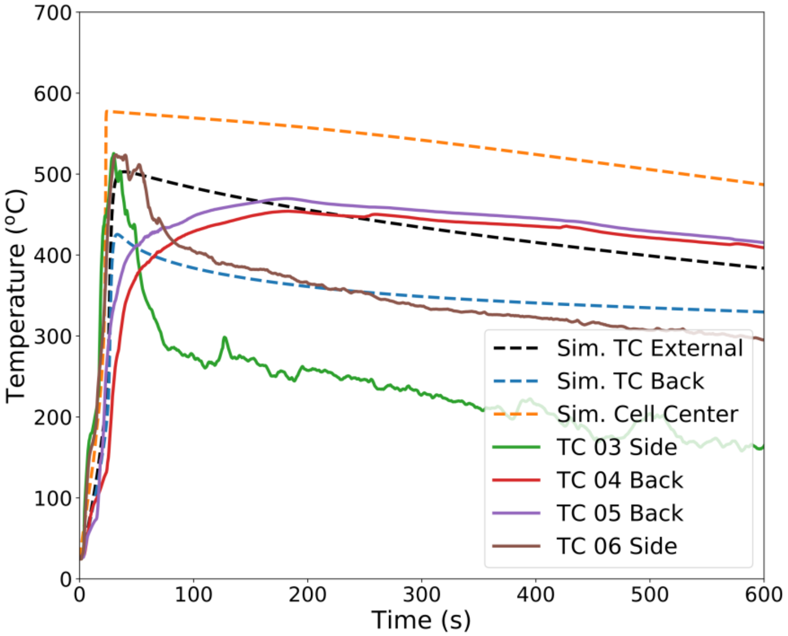
Large format prismatic cell demo: NITE collaboration nail penetration

Ongoing collaboration with NLAB at the National Institute of Technology and Evaluation in Japan.

- 100 Ah NMC prismatic cells
- Series of abuse tests with different initiation methods

LIM1TR simulations of nail penetration tests aid in interpreting the thermocouple measurements by understanding the heat transfer environment.



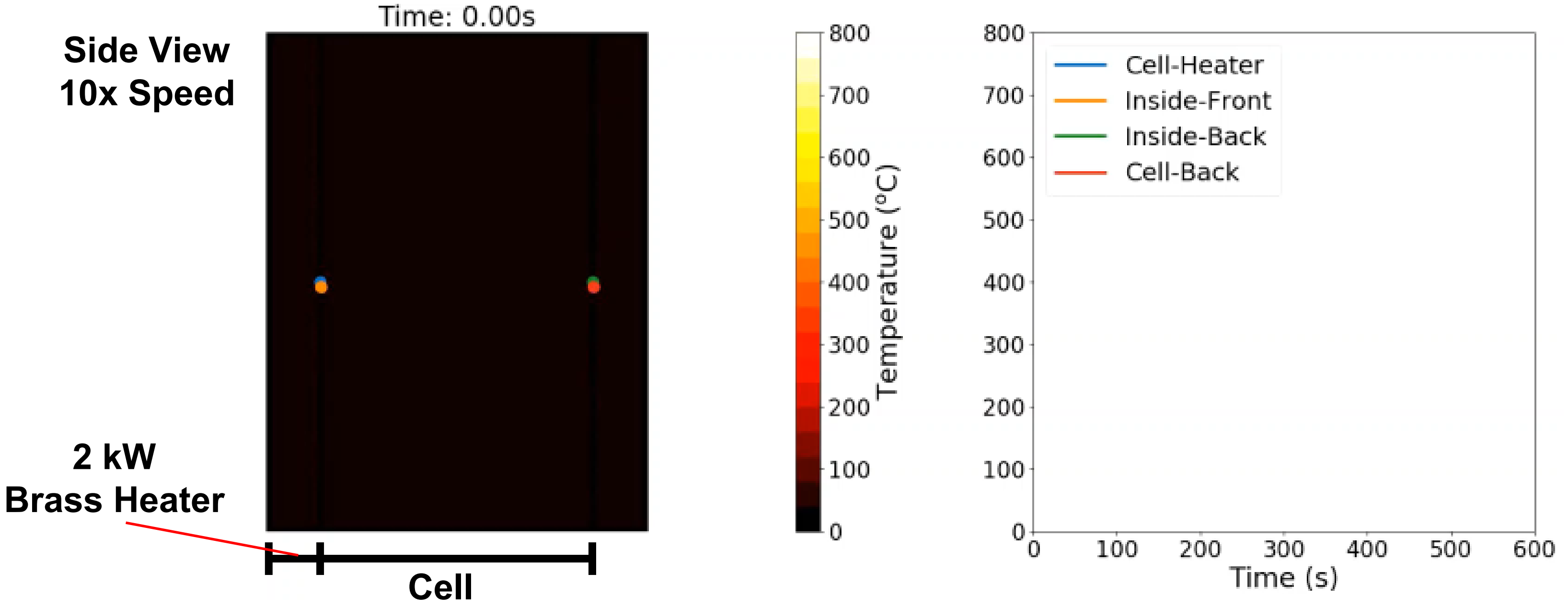


Large format prismatic cell: propagation test design for NITE collab.

Objective: initiate thermal runaway in a module of cells with a heat source.

What is the appropriate power for the heat source?

LIM1TR provides pre-test simulations to inform heater power selection.



Calibrating kinetics with calorimetry data

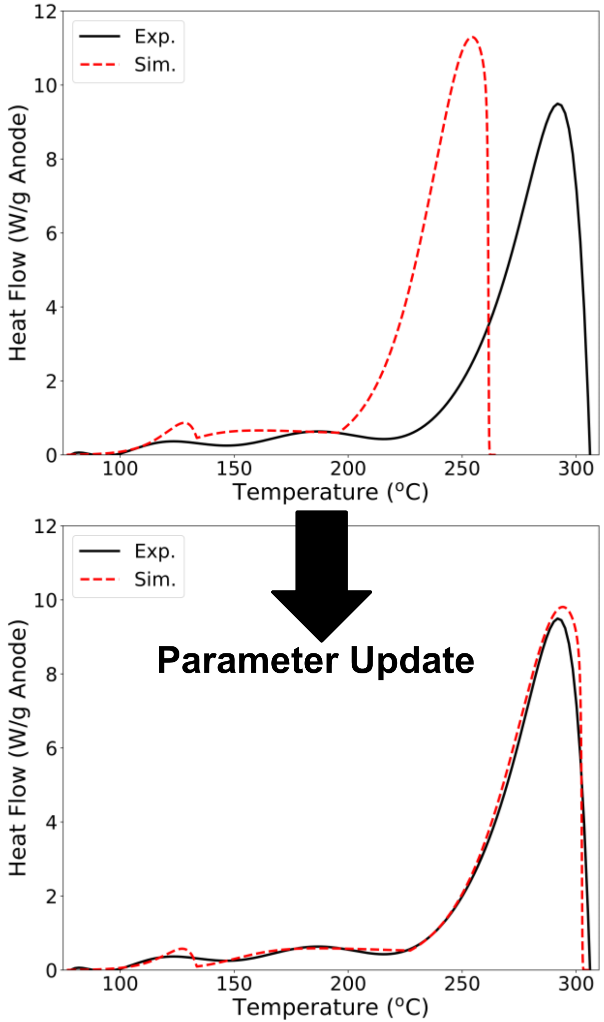
LIM1TR has a calorimetry mode for running differential scanning calorimetry (DSC) and accelerating rate calorimetry (ARC) simulations.

- Single control volume
- Fast computation time (~10s)

LIM1TR can be imported as a python module and connected to optimization software.

DSC example available on GitHub

- Critical thickness anode model
- Parameters in the input file can be updated with optimization tools for calibrating against experimental data
- Example shows effect of Arrhenius pre-exponential factor



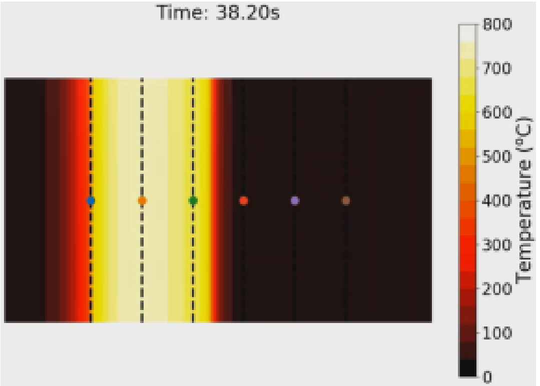
Summary

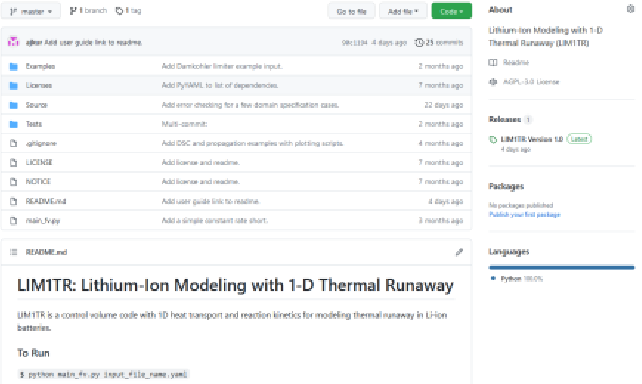
LIM1TR is an open source software package for simulating thermal runaway.

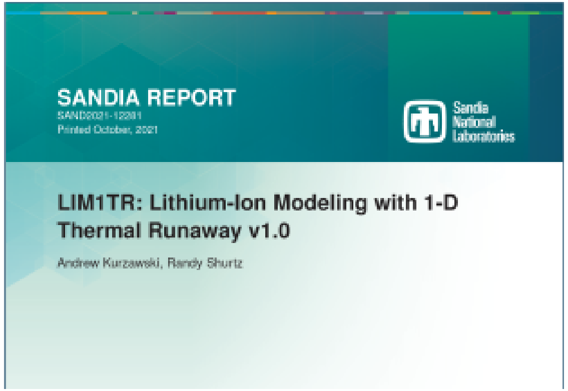
The software targets cascading thermal runaway predictions in module-scale and smaller systems.

The flexible user input allows for simulating a range of chemistries, module configurations, and external heating/abuse conditions.

We welcome users and collaborators! Please visit the GitHub repository (https://github.com/ajkur/lim1tr) to check out the code and read the user guide.







Acknowledgment

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Thanks to Joshua Lamb, Loraine Torres-Castro, and Alex Bates from Sandia National Labs for feedback on the code and user guide, as well as Ala’ Eyad Qatramez, Alexander Headley, and Daniel Foti from the University of Memphis for being early adopters of the beta version of the software.