# Thermal Abuse Simulation in a Battery

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# Agenda

- What is thermal abuse?
- Objectives of simulation
- Components (Models)
- Results

# What is thermal abuse?

Video found at https://www.ibtimes.com/tesla-news-model-s-crashes-tow-truck-russia-injuring-three-people-2812133

- **Exothermic** reaction within a battery cell
- Can quickly **propagate** to neighbor cells
- Does not need air to burn, hard to extinguish
- Can start by
  - Nail penetration
  - Internal short (dendrith growth)
  - External short
  - Crash
  - Thermal failures

https://www.ibtimes.com/tesla-news-model-s-crashes-tow-truck-russia-injuring-three-people-2812133

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# Objectives of simulation

- Does thermal runaway propagate to neighbor cells?
- How quickly does the propagation take place?
- Identify critical cells for start of thermal runaway
  - Reduce number of experiments
- What temperatures are reached, how much gas is released under what temperature and pressure?

# Components

- Nail model: Initiate the thermal runaway (in the lab, as a failure in the field)
- Internal short propagation (first mode of heat production)
- Thermal abuse model (1-eqn or NREL 4-eqn model)
- Gas release model
- Chemical reactions in gas/air mixture
- Boiling model of cooling liquid
- Particle release
- Damage modeling
  - Irreversible foam change
  - Melting
  - Deformation

# Components

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- Chemical reactions in gas/air mixture
- Boiling model of cooling liquid
- Particle release and tracking
- Damage modeling
  - Irreversible foam change
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  - Deformation

Todays talk, Workshop on ALH

Possible, but not tested yet for this application

# Components

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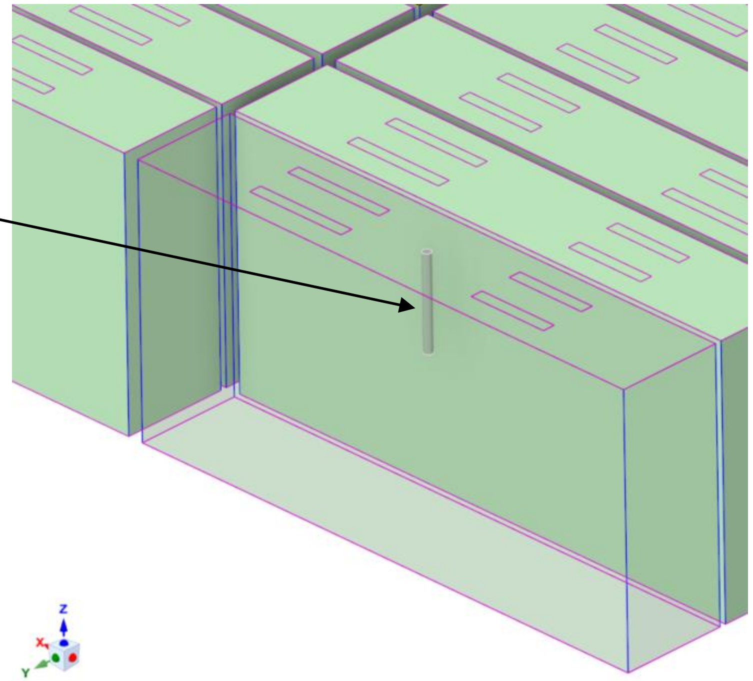
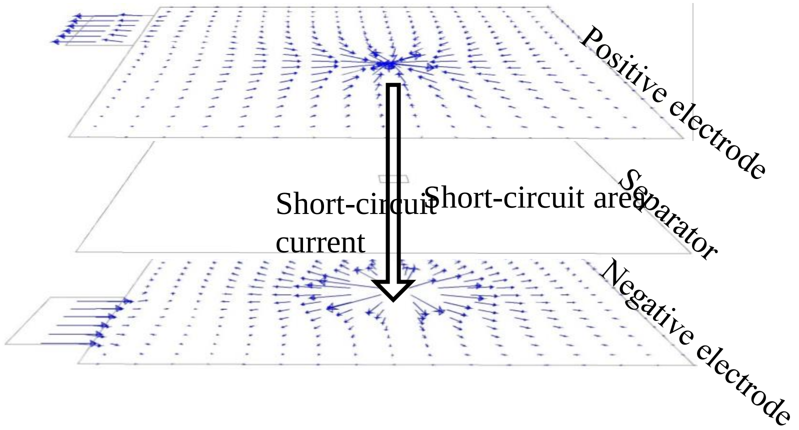
# Nail model

- Prepare in the battery geometry a small cylindrical region
- 2 different methods available:



- Heat source method
  - Apply for some time a heat source. Usually try and error to determine magnitude and duration. „just enough to start the thermal runaway“
- Specify internal short resistance
  - Would take into account the SOC
  - Non-trivial to find correct resistance
  - Requires to run dual-potential MSMD battery model



# Components

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# Internal short propagation

- Electric separator fails at temperatures lower than thermal abuse reactions
- Electric energy converted depends on (local) SOC
- Recommended: Reaction rate model (a 5th reaction similar to NREL 4 eqn model)
  - Does not require dual-potential MSMD model
  - Very efficient

$$R_{sh}(T, SoC) = ISC_{cond} \times A_{ec} \times \exp\left(-\frac{E_{ec}}{R_u T}\right) \times SoC$$

$$\frac{dSoC}{dt} = -R_{sh}$$

$$S_{ec} = H_{ec} \times R_{sh}$$

P. T. Coman, E. C. Darcy, C. T. Veje, and R. E. White, "Modelling Li-Ion Cell Thermal Runaway Triggered by an Internal Short Circuit Device Using an Efficiency Factor and Arrhenius Formulations", J. of the Electrochemical Society, 164 (4) A587-A593 (2017).

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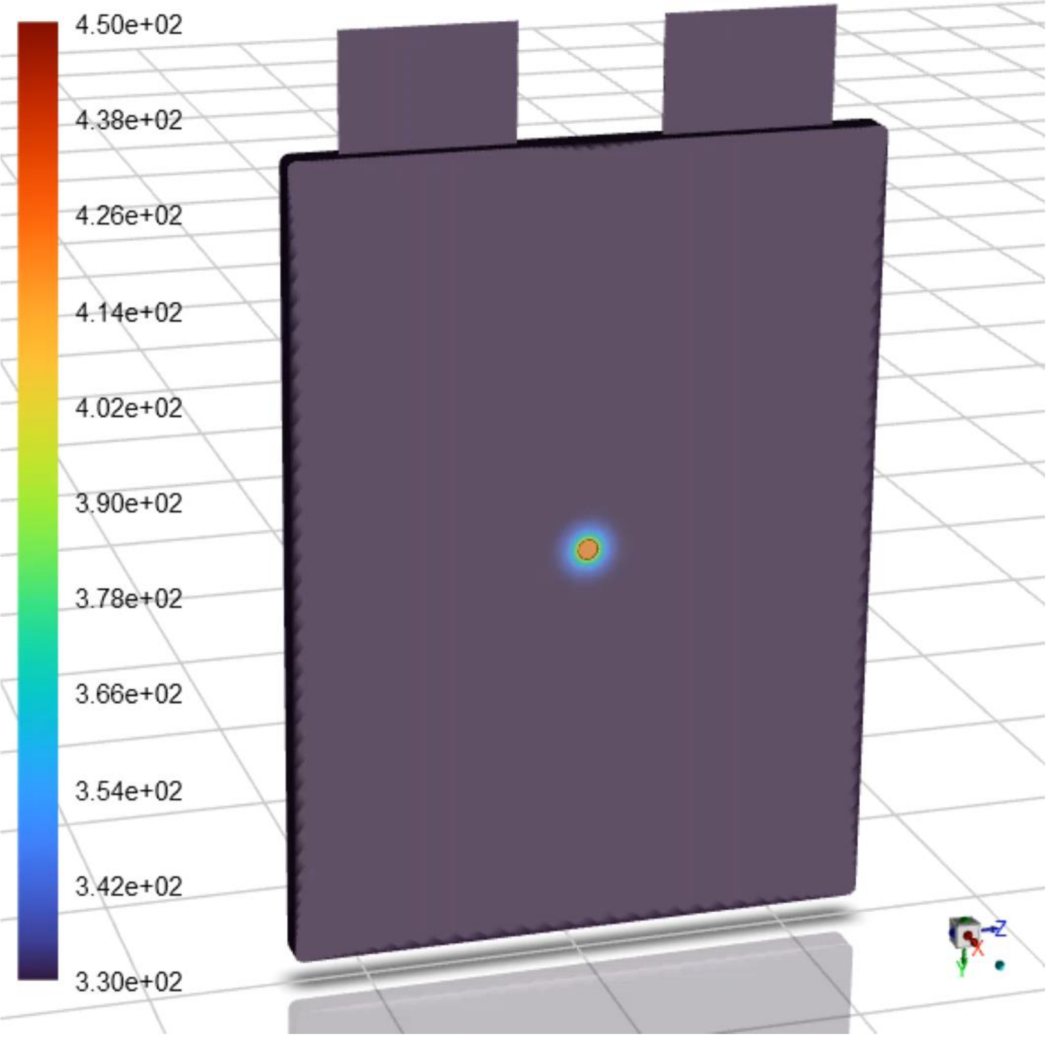
# Case03 – Short Propagation Animation



# Components

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# Introduction of Battery Thermal Abuse Models

- Reaction kinetics are used to model the decomposition reactions.
- Two models have been implemented in both Twin Builder and Fluent
  - **One-equation model**
    - D. D. MacNeil, J. R. Dahn, "Test of Reaction Kinetics Using Both Differential Scanning and Accelerating Rate Calorimetries as Applied to the Reaction of LixCoO2 in Non-aqueous Electrolyte", J. Phys Chem., 2001.
  - **NREL's four-equation model**
    - T. D. Hatchard, D. D. MacNeil, A. Basu, and J. R. Dahn, "Thermal Model of Cylindrical and Prismatic Lithium-Ion Cells", J. of the Electrochemical Society, 2001.
    - Gi-Heon Kim, Ahmad Pesaran, Robert Spotnitz, "A Three-dimensional thermal abuse model for lithium-ion cells", J. of Power Resources, 2007.

# 1-Eqn Thermal Abuse Model

- Total heat generation due to thermal abuse can be modeled as one exothermic reaction.

$$S_{abuse\_chem} = S$$

$$R(T,\alpha) = A \times \alpha^m \times (1-\alpha)^n \times \exp\left(-\frac{E_a}{R_u T}\right)$$

$$S = H \times W \times R$$

$$\frac{d\alpha}{dt} = R$$

where A, m, n, $E_a$, H, W are model constants; H specific heat (J/kg); W volume specific content (kg/m^3)

- This is a sub-set of the 4-equ thermal abuse model.

| | reaction model | $d\alpha/dt =$ | $k\alpha^m(1-\alpha)^n(-\ln(1-\alpha))^p$ m | n | P |
|---|---|---|---|---|---|
| 1 | one-dimensional diffusion | $k\alpha^{-1}$ | −1 | 0 | 0 |
| 2 | | $k\alpha$ | 1 | 0 | 0 |
| 3 | power law | $k\alpha^{1/2}$ | 0.5 | 0 | 0 |
| 4 | power law | $k\alpha^{2/3}$ | 2/3 | 0 | 0 |
| 5 | power law | $k\alpha^{3/4}$ | 3/4 | 0 | 0 |
| 6 | zero order | k | 0 | 0 | 0 |
| 7 | contracting cylinder | $k(1-\alpha)^{1/2}$ | 0 | 0.5 | 0 |
| 8 | contracting sphere | $k(1-\alpha)^{2/3}$ | 0 | 2/3 | 0 |
| 9 | first order ($n^{th}$ order) | $k(1-\alpha)$ | 0 | 1 | 0 |
| 10 | second order ($n^{th}$ order) | $k(1-\alpha)^2$ | 0 | 2 | 0 |
| 11 | Avrami−Erofeev | $k(1-\alpha)(-\ln(1-\alpha))^{1/2}$ | 0 | 1 | 0.5 |
| 12 | Avrami−Erofeev | $k(1-\alpha)(-\ln(1-\alpha))^{2/3}$ | 0 | 1 | 2/3 |
| 13 | Avrami−Erofeev | $k(1-\alpha)(-\ln(1-\alpha))^{3/4}$ | 0 | 1 | 3/4 |
| 14 | autocatalytic | $k\alpha(1-\alpha)$ | 1 | 1 | 0 |
| 15 | two-dimensional diffusion | $k(-\ln(1-\alpha))^{-1}$ | 0 | 0 | −1 |
| 16 | diffusion controlled | $k(1-(1-\alpha)^{1/3})^{-1}(1-\alpha)^{2/3}$ | | | |
| 17 | diffusion controlled | $k((1-\alpha)^{-1/3}-1)^{-1}$ | | | |

D. D. MacNeil, J. R. Dahn, "Test of Reaction Kinetics Using Both Differential Scanning and Accelerating Rate Calorimetries as Applied to the Reaction of LixCoO2 in Non-aqueous Electrolyte", J. Phys Chem., 2001.

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# NREL's 4-Equ Thermal Abuse Model

**Table 1. Abuse reactions included in NREL's abuse reaction kinetics model**

| Reaction # | Reaction | Possible Onset Temperature (°C) |
|---|---|---|
| 1 | Solid Electrolyte Interphase (SEI) layer decomposition | 80 |
| 2 | Anode — electrolyte | 100 |
| 3 | Cathode — electrolyte | 130 |
| 4 | Electrolyte decomposition | 180 |

$$S_{abuse\_chem} = S_{sei} + S_{ne} + S_{pe} + S_{ele}$$

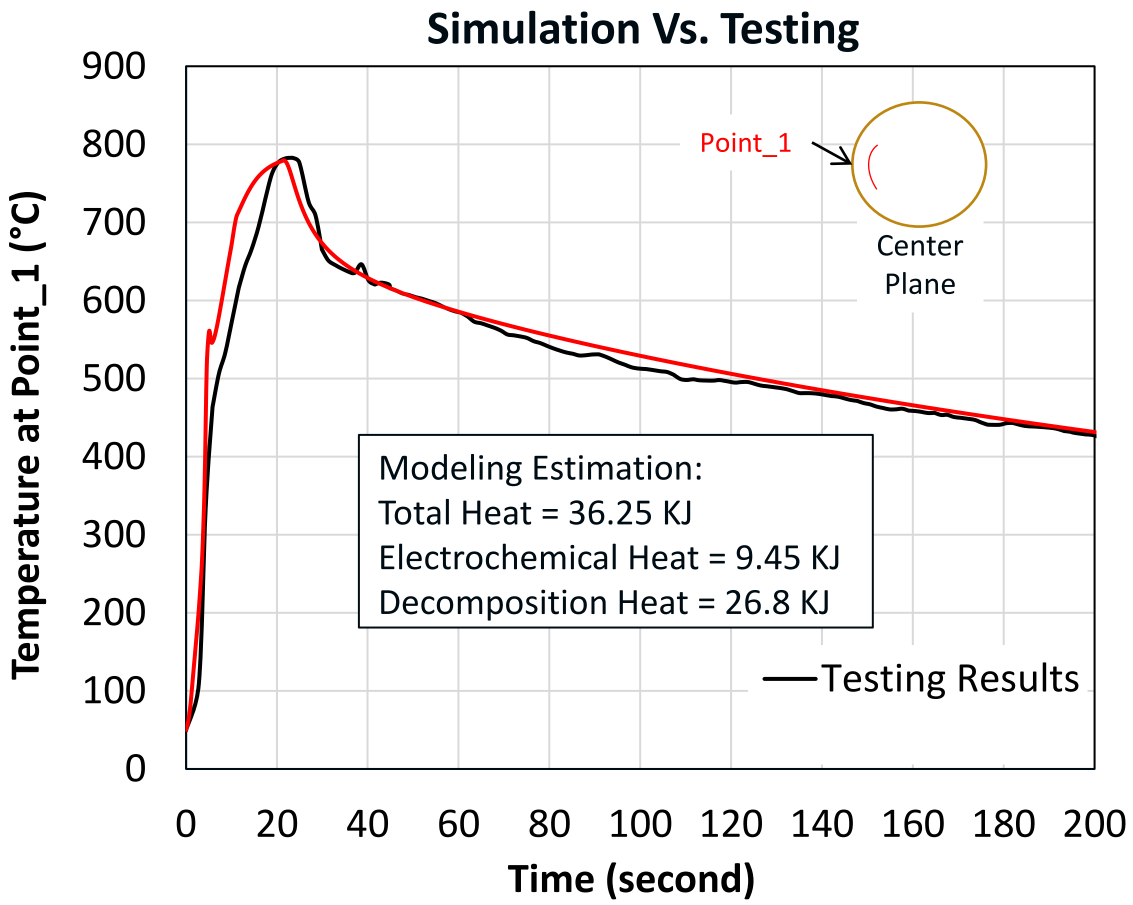
$$R_{sei}(T, c_{sei}) = A_{sei} \times \exp\left(-\frac{E_{a,sei}}{R_u T}\right) \times c_{sei}^{m_{sei}}$$

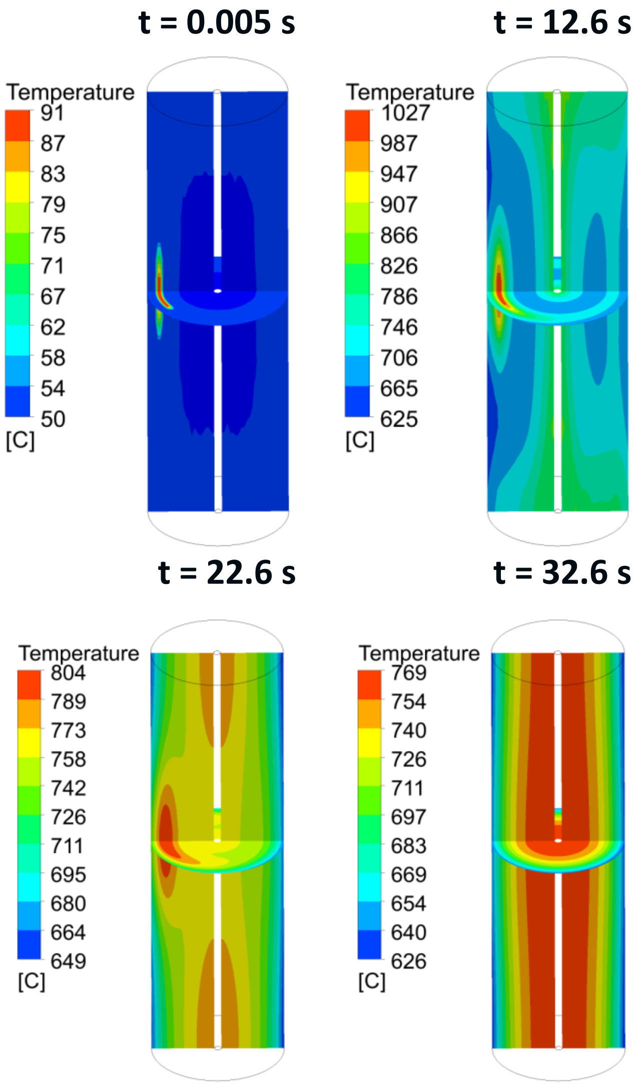
$$S_{sei} = H_{sei} \times W_c \times R_{sei}$$

$$\frac{dc_{sei}}{dt} = -R_{sei}$$

Gi-Heon Kim, Ahmad Pesaran, Robert Spotnitz, "A Three-dimensional thermal abuse model for lithium-ion cells", J. of Power Resources, 2007.

# Cell Thermal Runaway Validation



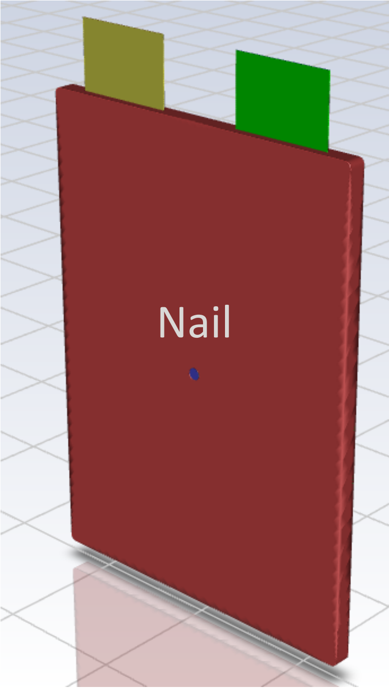



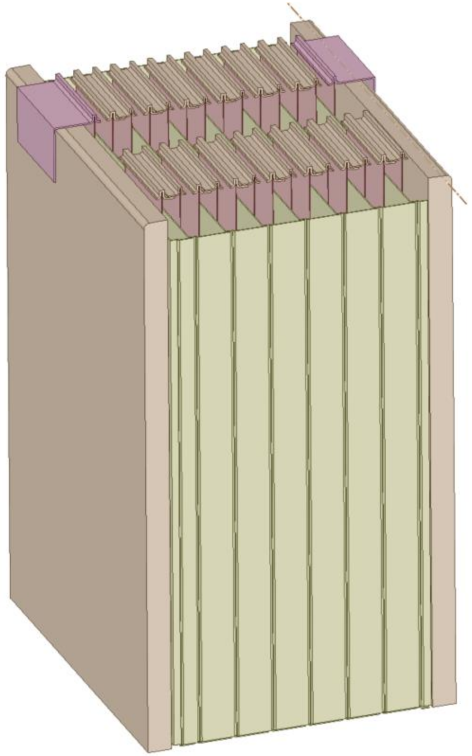

- The thermal conductivity within battery cell is anisotropy, which is 27 W/m-K, 27 W/m-K and 0.8 W/m-K in axial, azimuthal and radial directions, respectively
- Heat transfer rate along azimuthal and axial directions is faster than radial direction

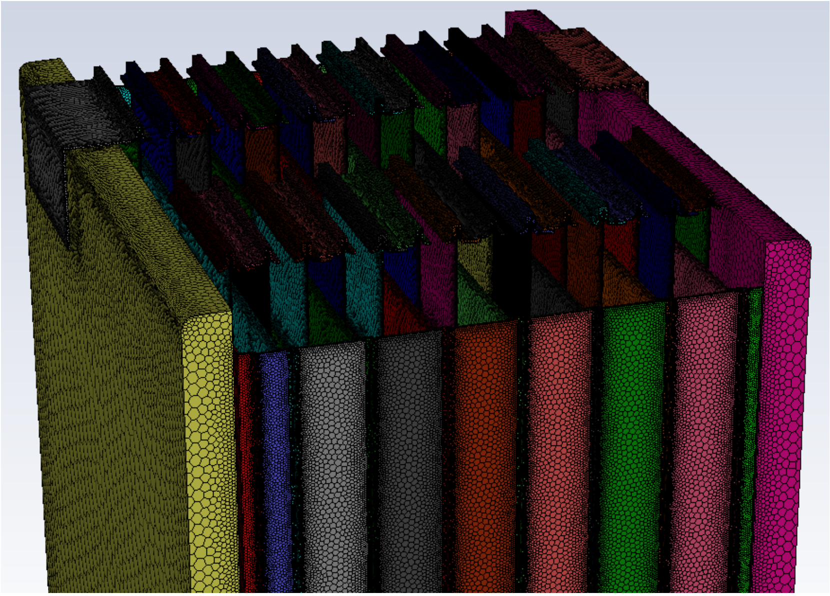

1. "Numerical Investigation of Thermal Runaway Propagation Induced By Internal Short Circuits in a Li-Ion Battery Module", 231st ECS Meeting, New Orleans, LA, May 2017.

# ALH Tutorial

- The thermal runaway propagation will be performed on a module of 14 cells.
  - The nail region is at the center of the first cell.
- The geometry and the mesh is shown here.
  - The module mesh consists of 4.0 M polyhedral cells.

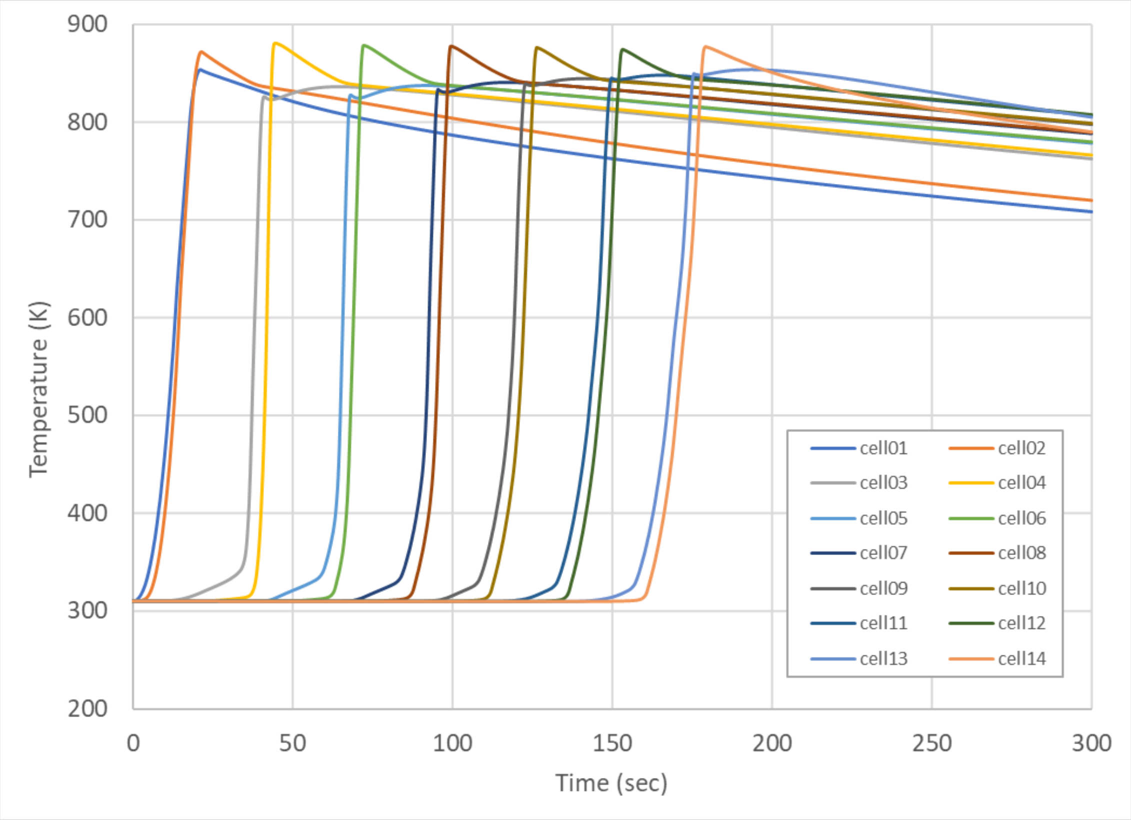


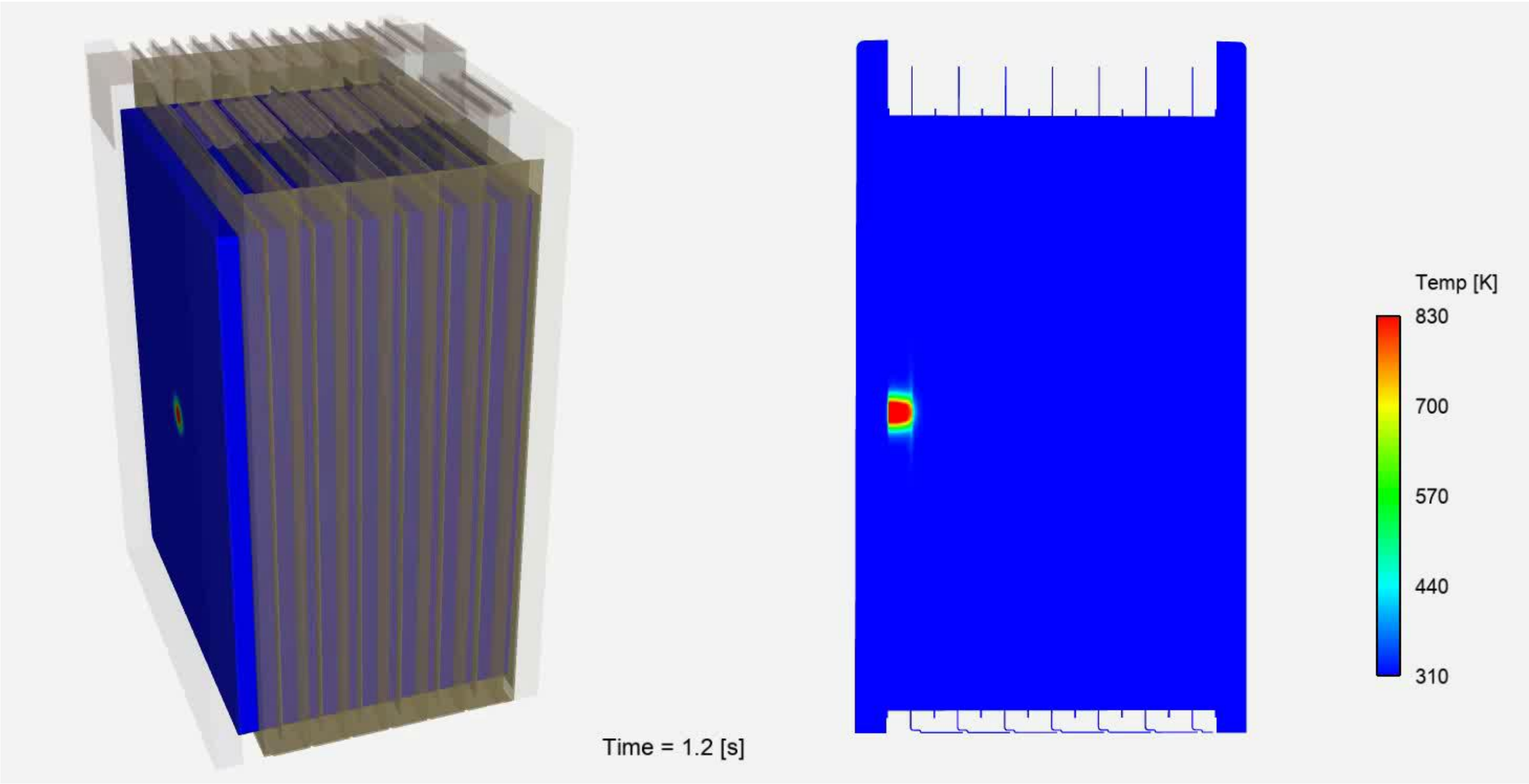


# Thermal Runaway Propagation

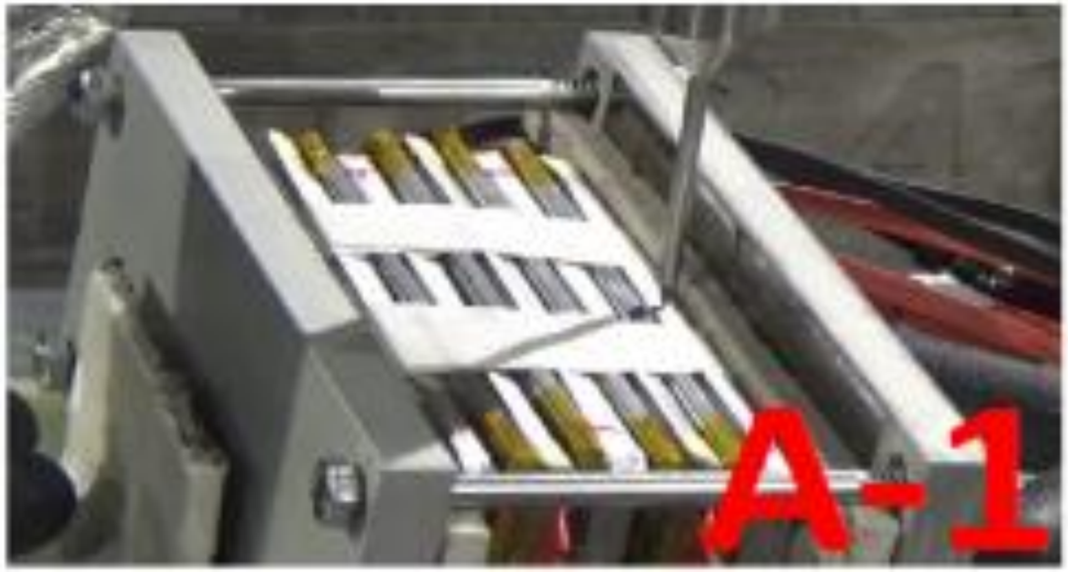
- 14 cells in the module
- A pair of two cells shares a cooling fin.
- Thermal runaway propagates from one pair of cells to another.
- One of the design goals is to prevent such propagation.



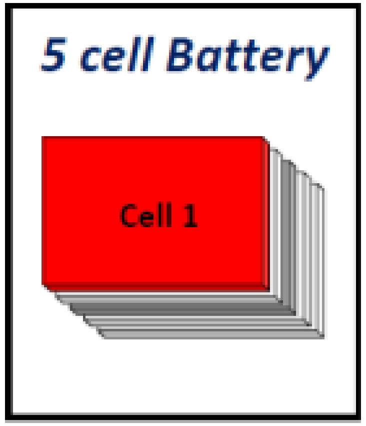
# Thermal Runaway Animation

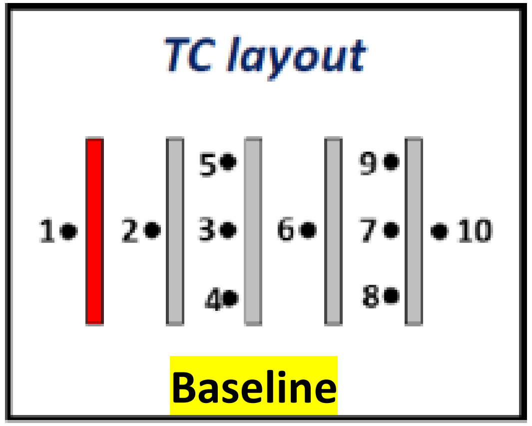


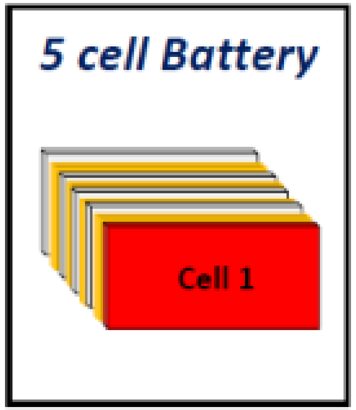
# Thermal Runaway Propagation Validation

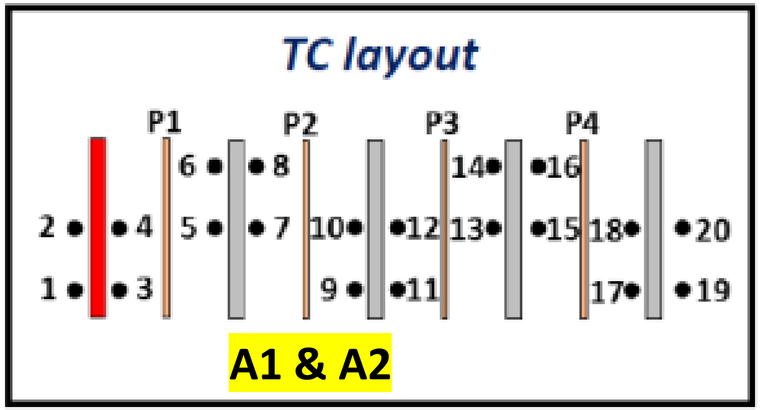



| Case No. | Testing Description |
|---|---|
| Baseline | No thermal management |
| A1 | 3.2 mm Al plates between Cells |
| A2 | 0.8 mm Al plates between Cells |



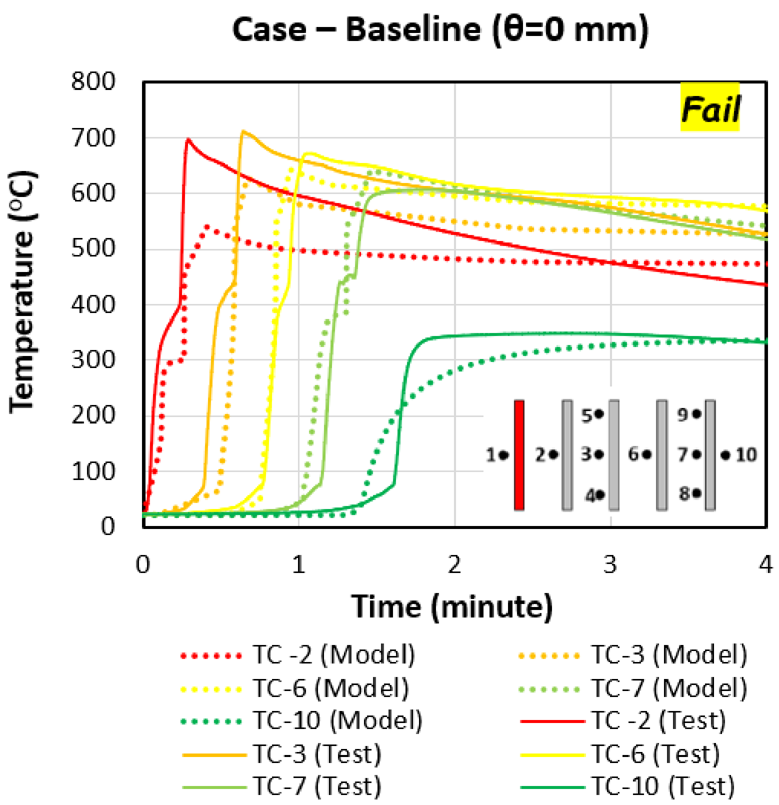



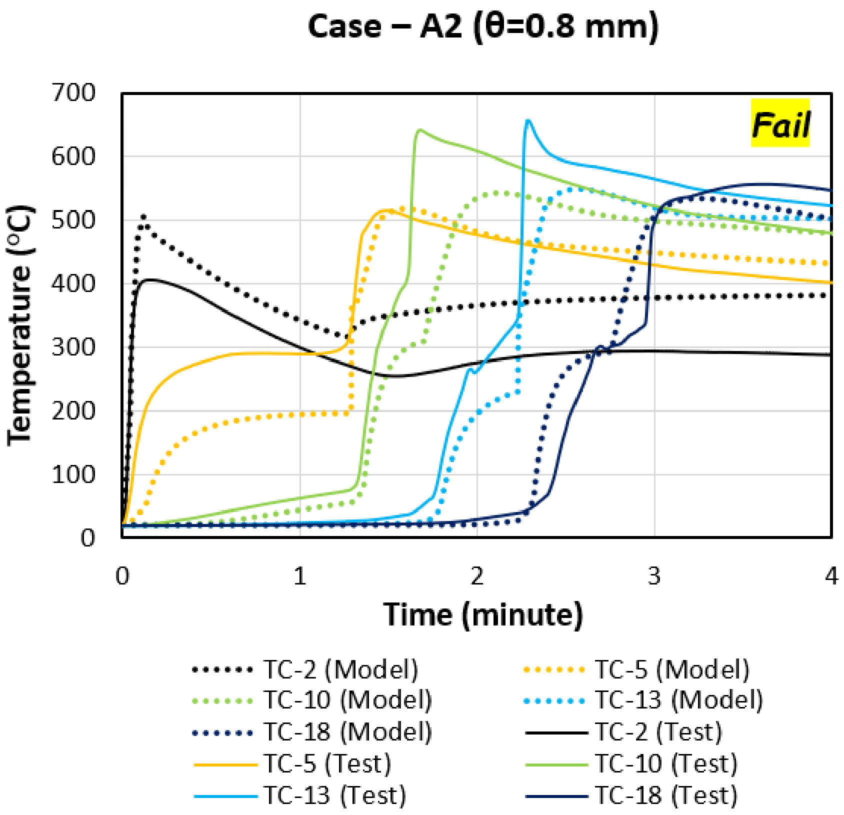




2. Q Li, CB Yang, S. Santhanagopalan, K. Smith, J. Lamb, L. Steele, L. Torres-Castro, "Numerical Investigation of Thermal Management for Lithium-ion Battery Pack under Thermal Abuse Condition, J. Power Sources429 (2019) 80-88

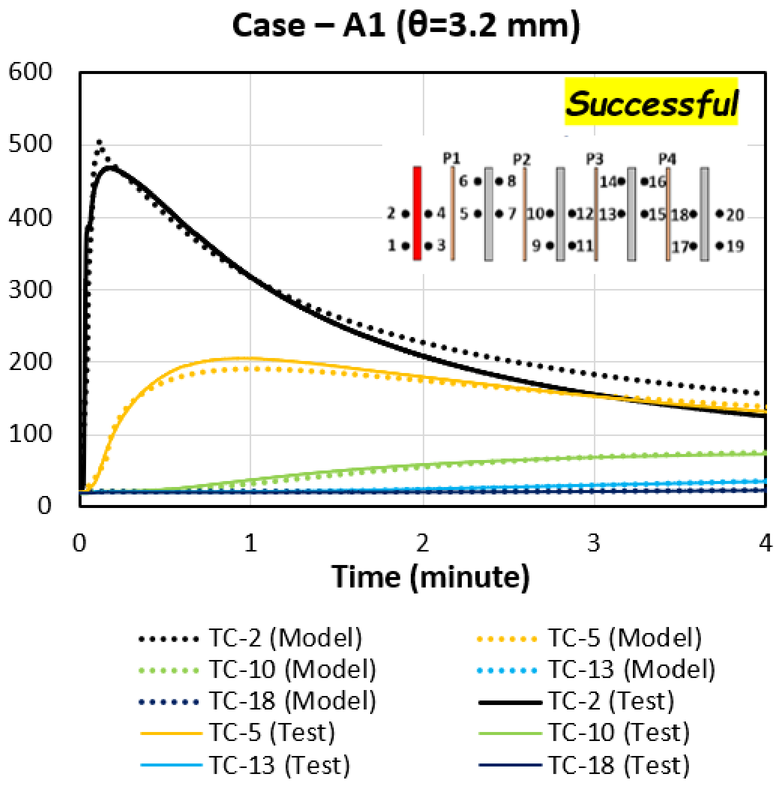
# Thermal Runaway Propagation Validation




Baseline




0.8 mm Al-sheet




3.2 mm Al-sheet

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# Components

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# Gas release (venting) model

- The released gas has properties of **hot air**, but is traced as venting-gas, which allows to determine an air to venting-gas ratio in the domain
  - The assumption is that all **oxygen in the battery** is very quickly replaced or consumed
- The total **amount** of gas set free for each cell is **user supplied**
- The current **mass flow rate** of gas is calculated from the **rate of change of the electrolyte reaction** in the corresponding active cell zone
- The temperature of the hot air is the **average cell temperature**
- The best run-time performance of this is obtained by using a user defined function (**UDF**)

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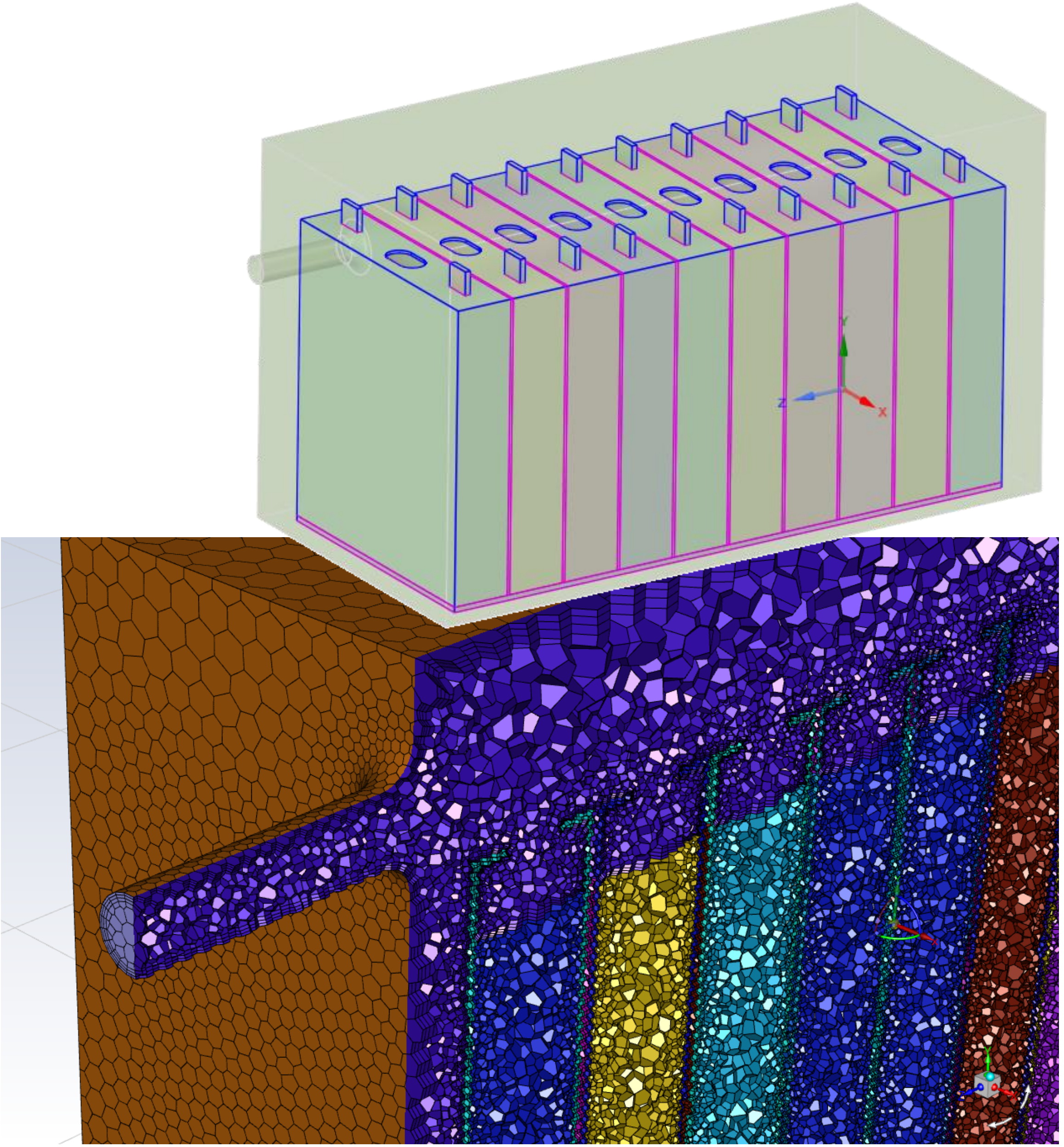
# Foam destruction

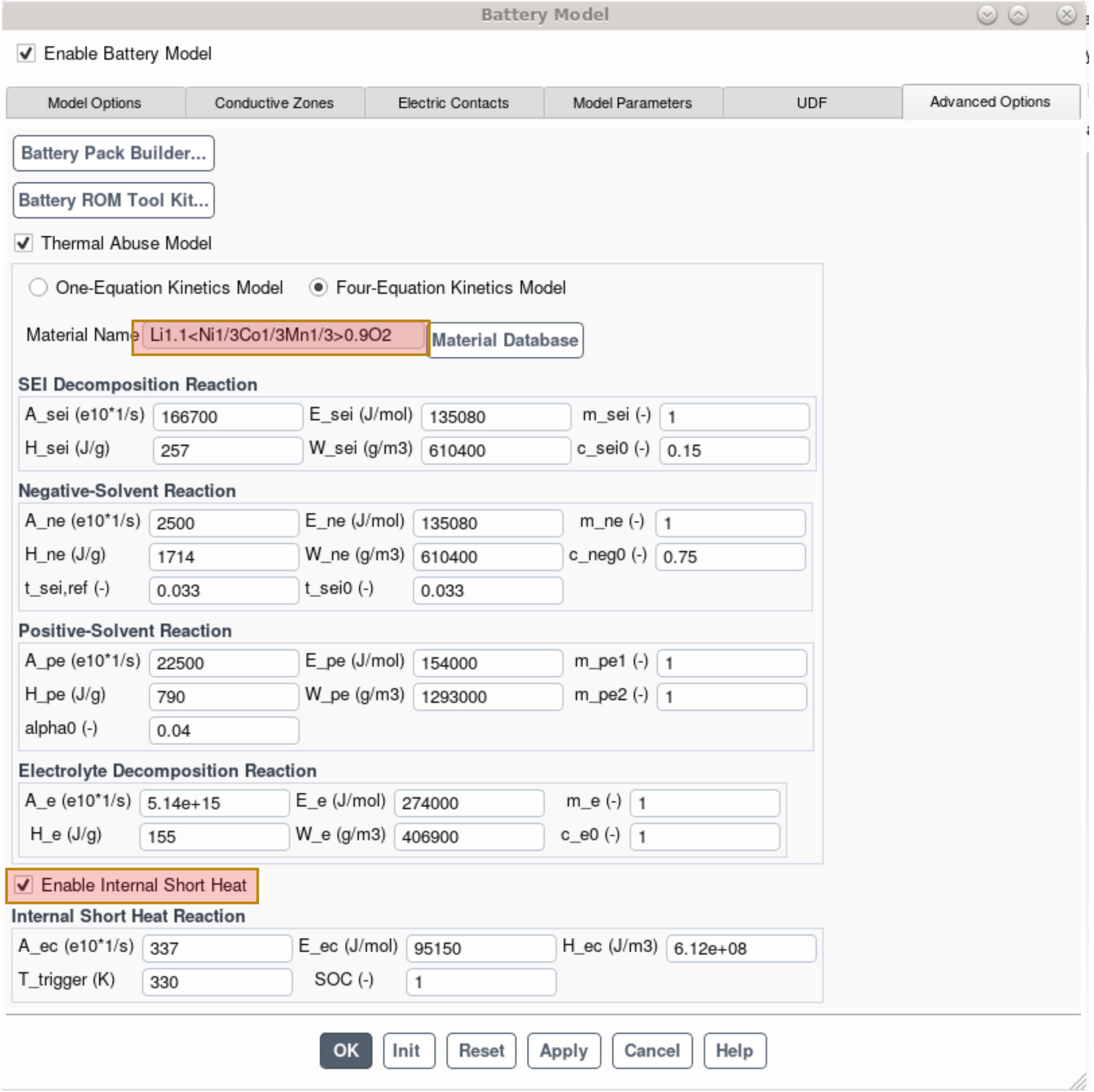
- Foam is transformed to a coal like solid
- If T>200°C, foam gets permanently a higher thermal conductivity
- State is tracked in User Defined Memory (UDM), property of each finite-volume cell
- Implemented as a User Defined Function (UDF)

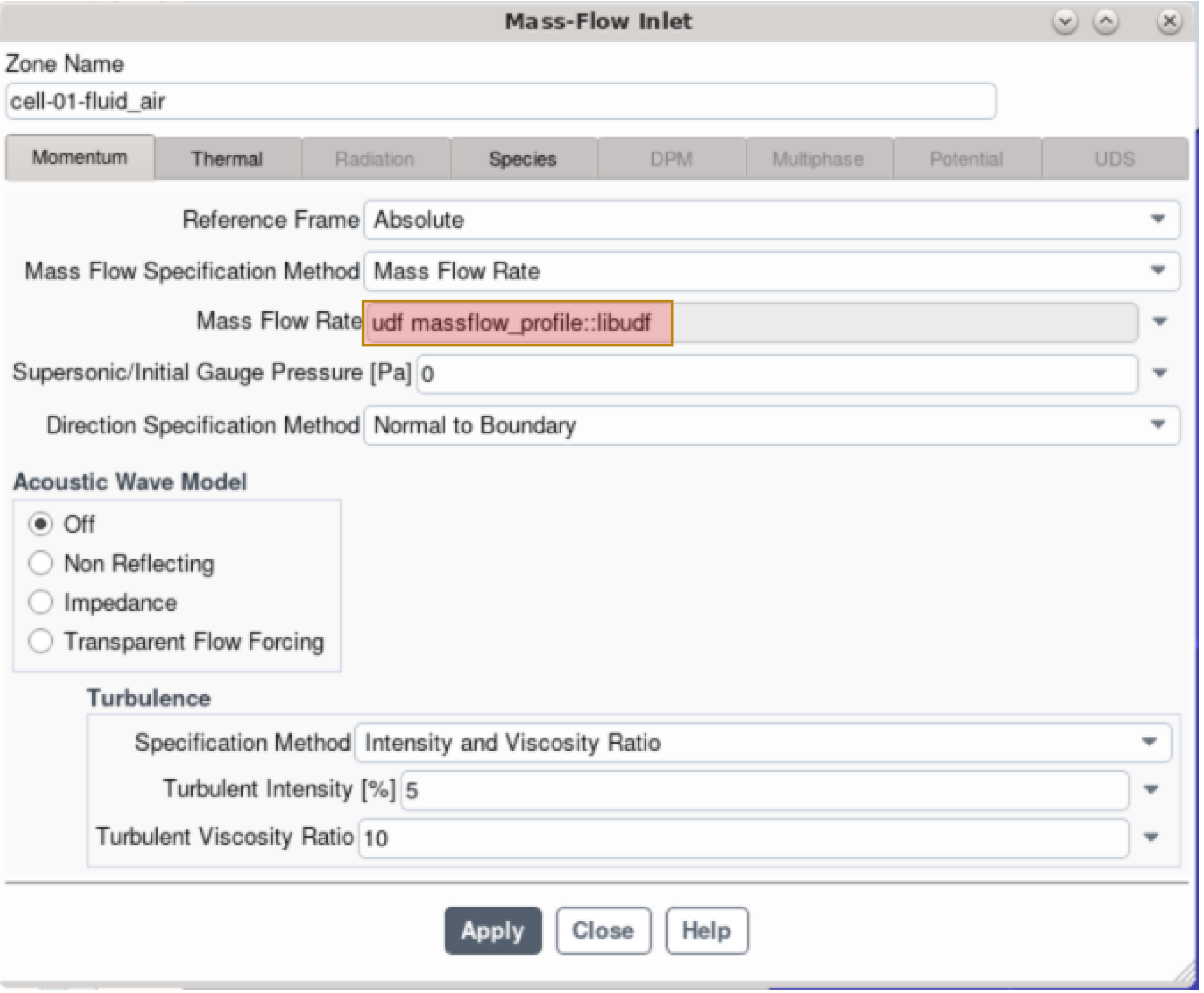
# New tutorial on ALH

- Uses all features presented so far
  - Initiate thermal runaway with nail region
  - Internal short circuit propagation
  - NREL 4-eqn model
  - Gas release
  - Irreversible foam change
- 10 prismatic battery cells
- 3.3 mio prism polyhedra cells
- Time step 0.025 s, 800 time steps, 20 s total
- 21 h on 32 cores
- Overnight on 128 cores



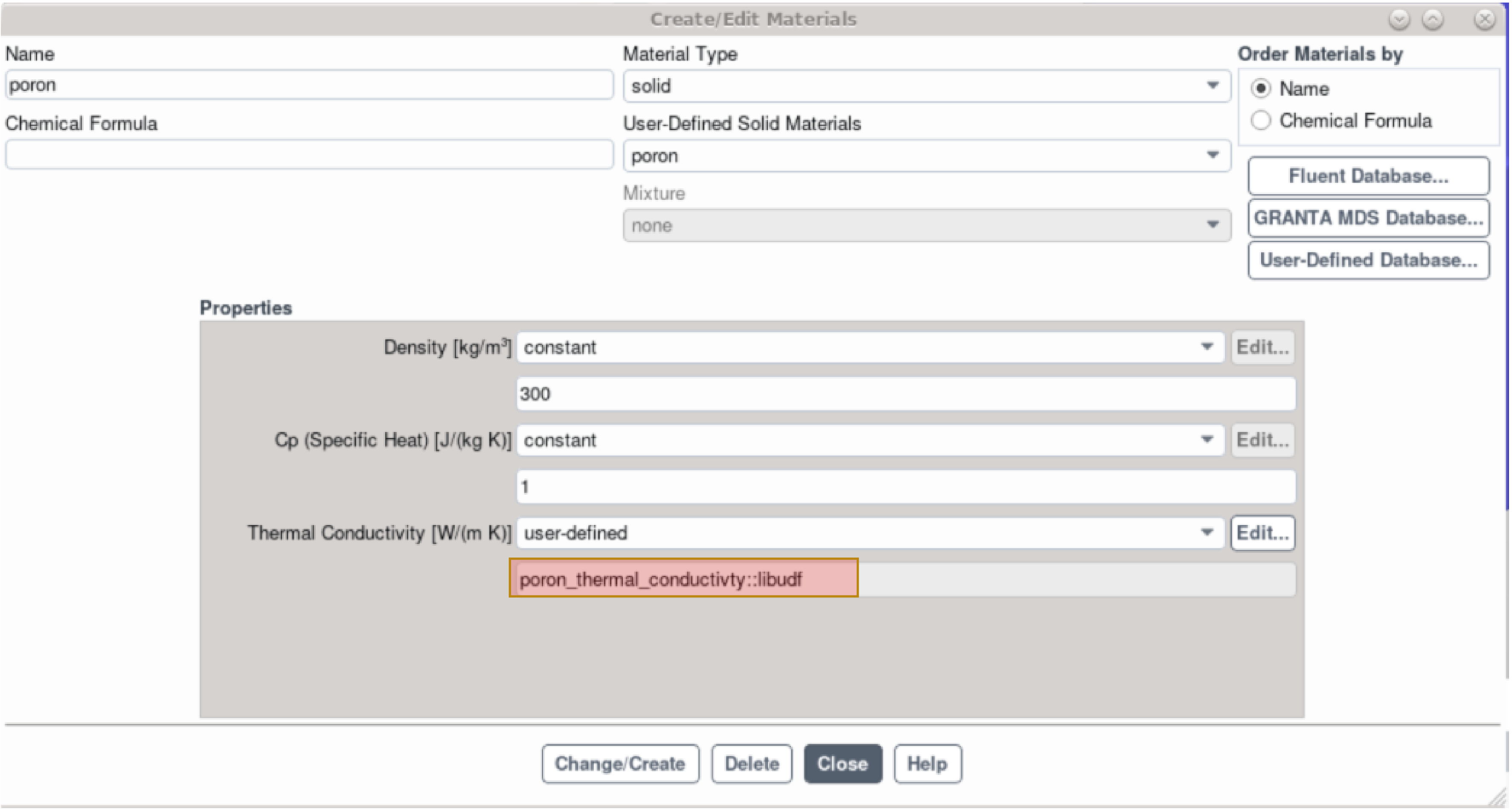
# Thermal Abuse Model



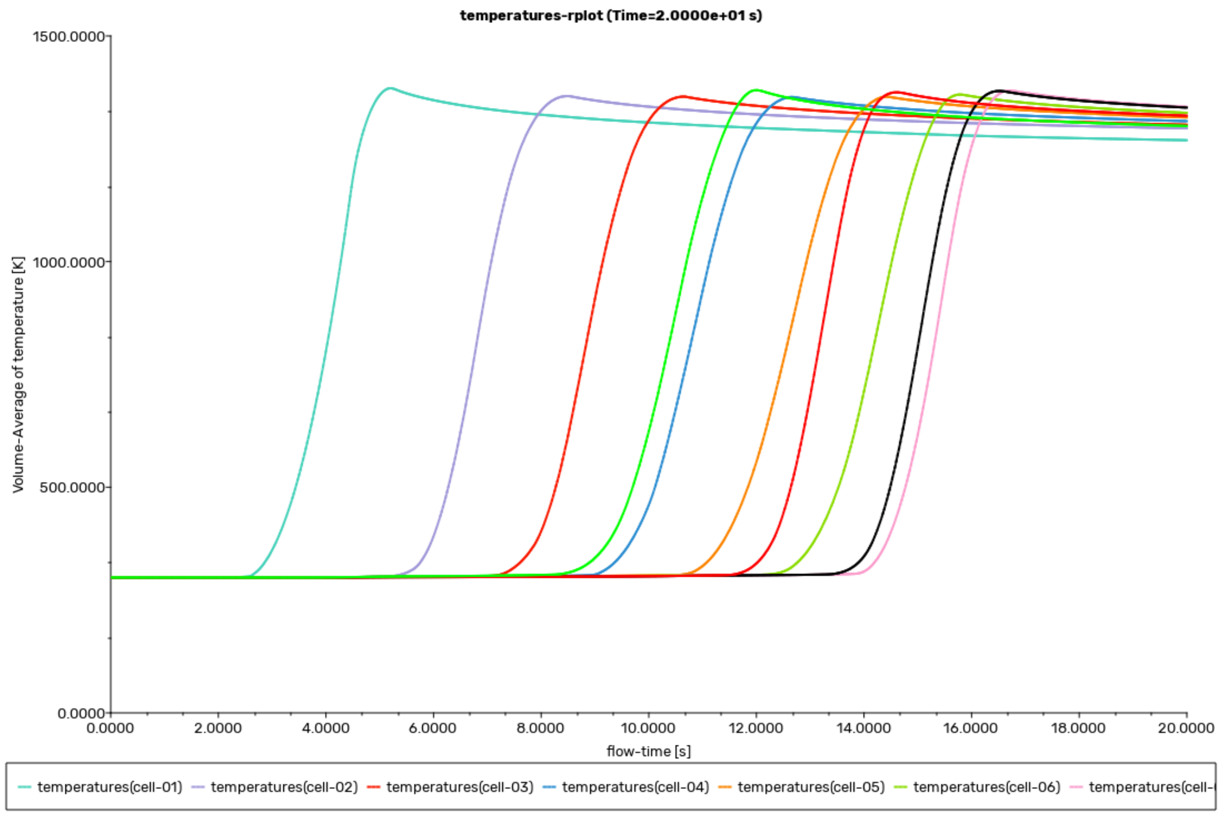



# Poron with non-reversible material property

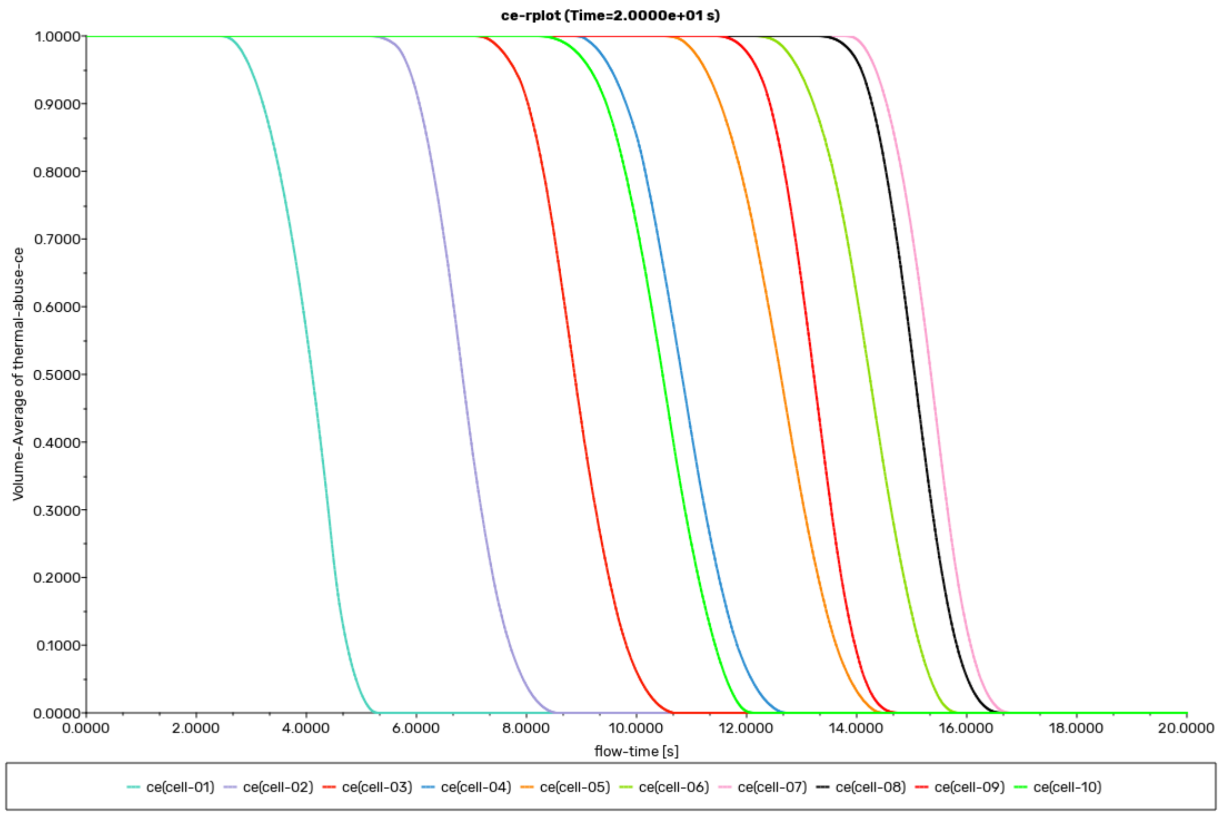
- Activate 1 user defined memory (UDM)
- Hook UDF for thermal conductivity



# Monitors

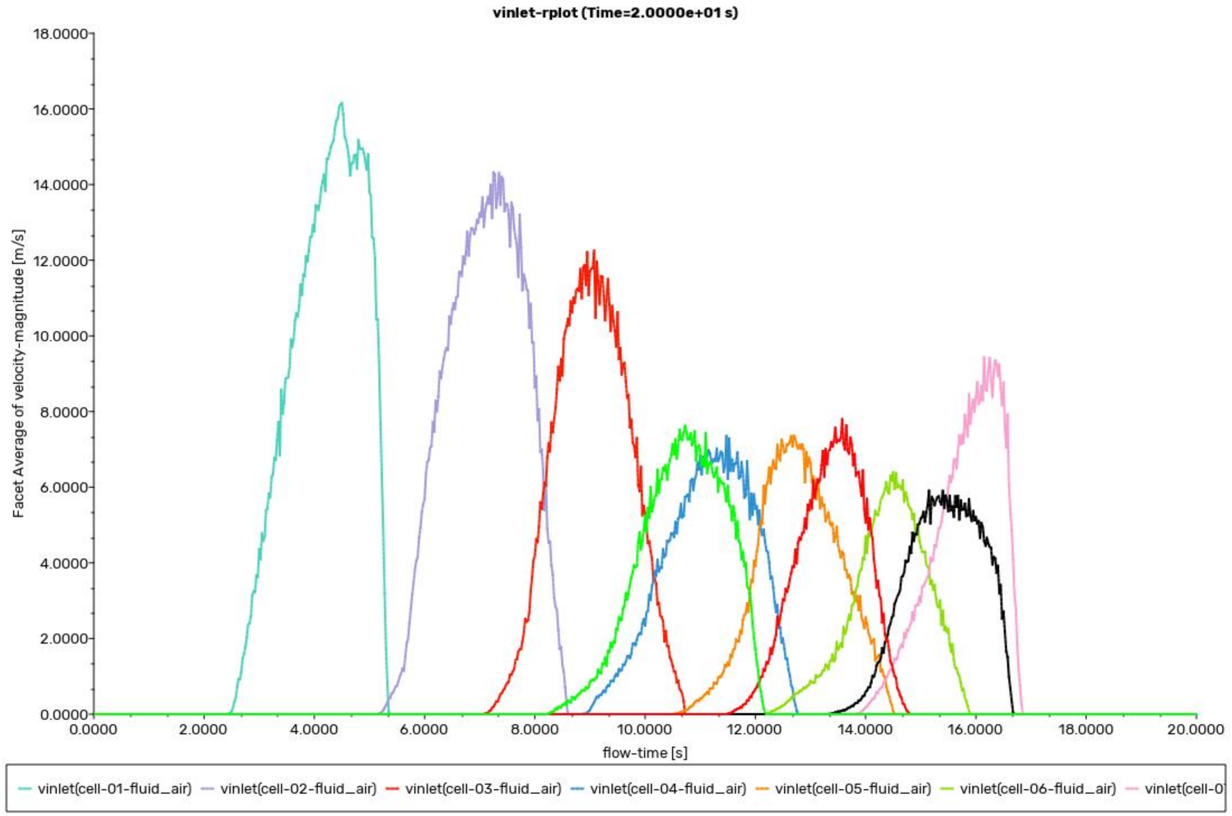


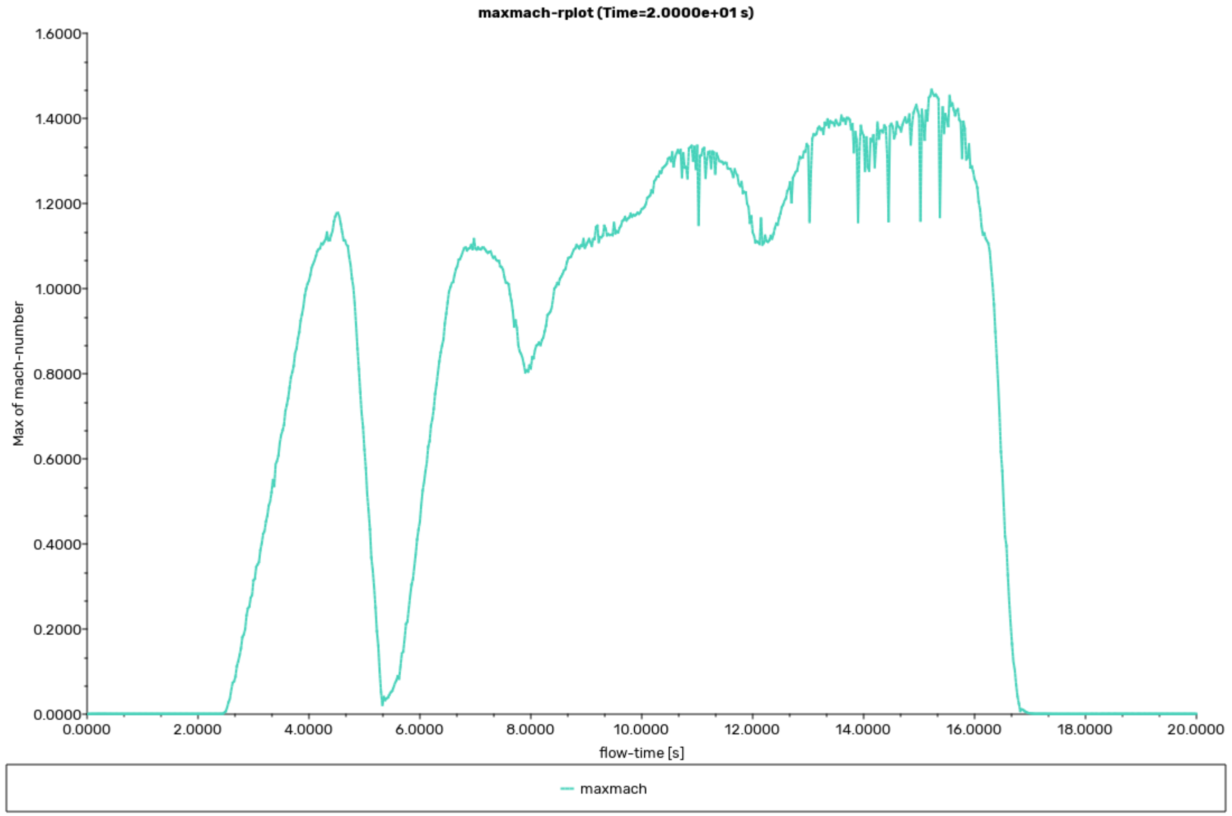
temperatures-rplot (Time=2.0000e+01 s)
Volume-Average of temperature [K]
1500.0000
1000.0000
500.0000
0.0000
0.0000
2.0000
4.0000
6.0000
8.0000
10.0000
12.0000
14.0000
16.0000
18.0000
20.0000
flow-time [s]
temperatures(cell-01)
temperatures(cell-02)
temperatures(cell-03)
temperatures(cell-04)
temperatures(cell-05)
temperatures(cell-06)

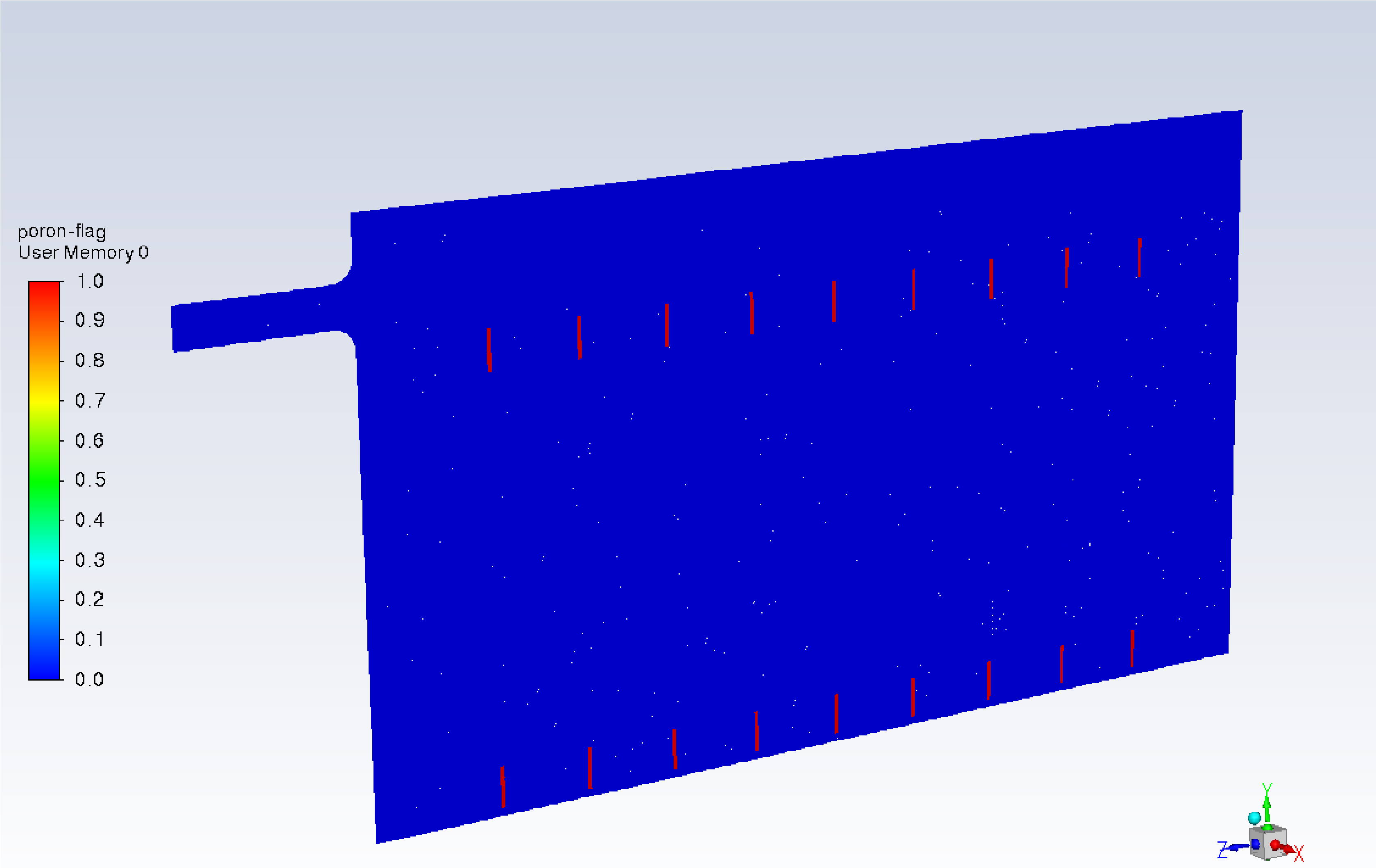
ce-rplot (Time=2.0000e+01 s)
Volume-Average of thermal-abuse-ce
1.0000
0.9000
0.8000
0.7000
0.6000
0.5000
0.4000
0.3000
0.2000
0.1000
0.0000
0.0000
2.0000
4.0000
6.0000
8.0000
10.0000
12.0000
14.0000
16.0000
18.0000
20.0000
flow-time [s]
ce(cell-01)
ce(cell-02)
ce(cell-03)
ce(cell-04)
ce(cell-05)
ce(cell-06)
ce(cell-07)
ce(cell-08)
ce(cell-09)
ce(cell-10)

# Monitors


vinlet-rplot (Time=2.0000e+01 s)
Facet Average of velocity-magnitude [m/s]
flow-time [s]
vinlet(cell-01-fluid_air)
vinlet(cell-02-fluid_air)
vinlet(cell-03-fluid_air)
vinlet(cell-04-fluid_air)
vinlet(cell-05-fluid_air)
vinlet(cell-06-fluid_air)
vinlet(cell-0

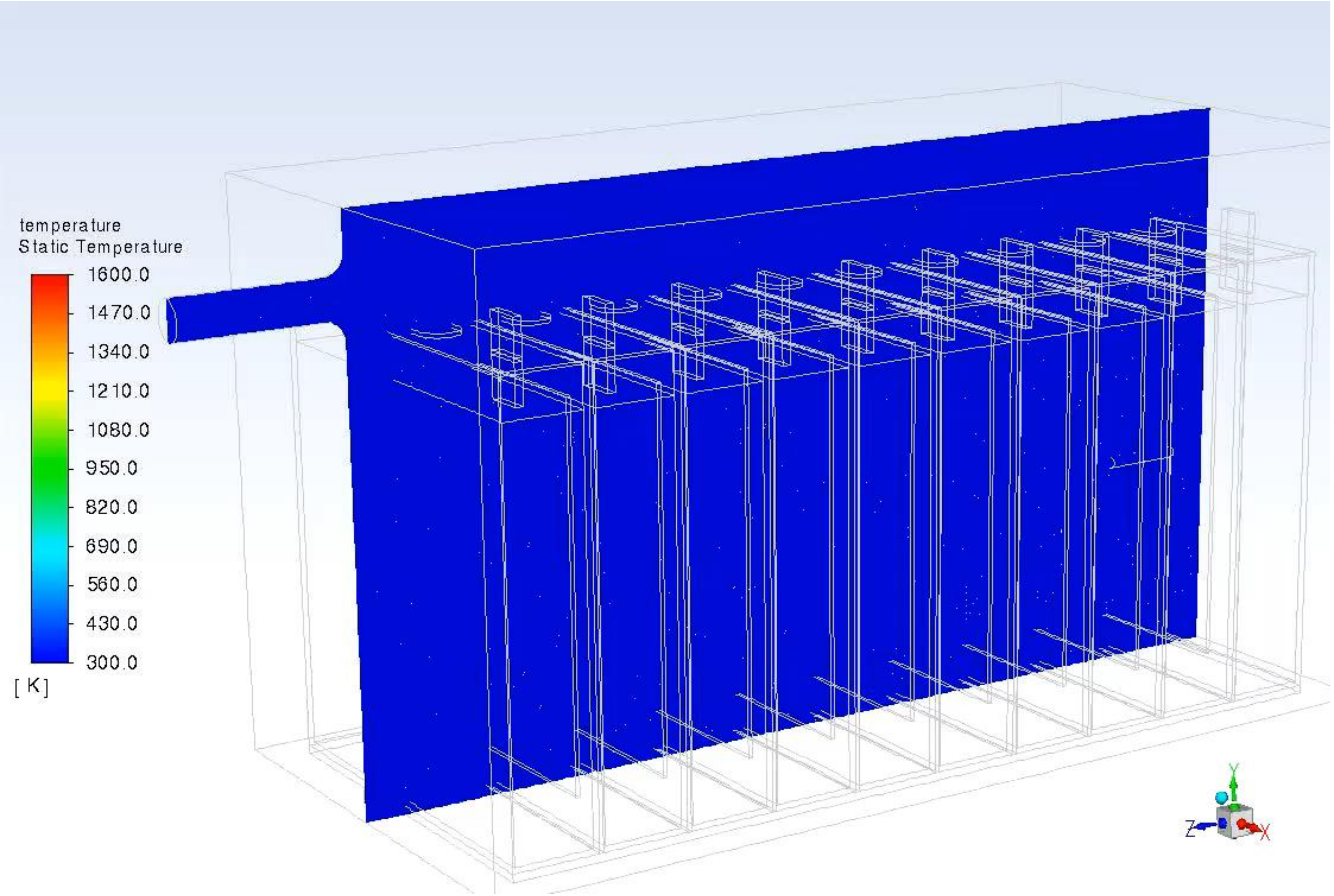

maxmach-rplot (Time=2.0000e+01 s)
Max of mach-number
flow-time [s]
maxmach

# Poron non-reversible change




The flag for poron change is activated in all 9 regions

# Animation



temperature
Static Temperature
1600.0
1470.0
1340.0
1210.0
1080.0
950.0
820.0
690.0
560.0
430.0
300.0
[ K ]
Y
Z
X

# Manage Thermal Runaway

## Customer Goals

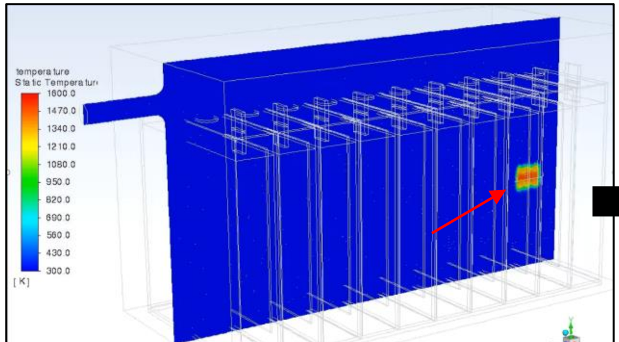
- Ensure that a **thermal runaway event will stay within regulatory limits.**
- **Reduce development time and costs** by replacing expensive measurements with simulation.

## Solution

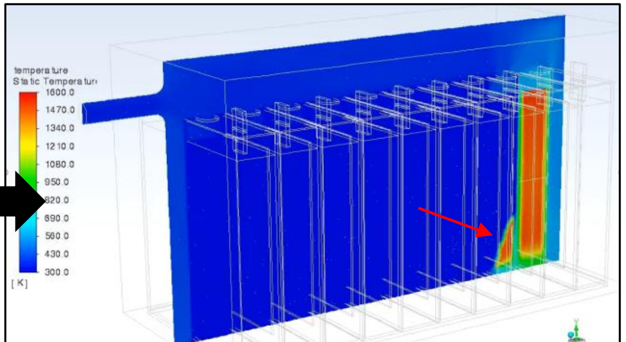
- **Heat sources and thermal conduction are modeled with build-in models of Ansys Fluent**
- **Gas release from cells is captured with a UDF** which relates the reaction progress in each cell with a mass flow inlet at the venting holes of the cells

## Benefits

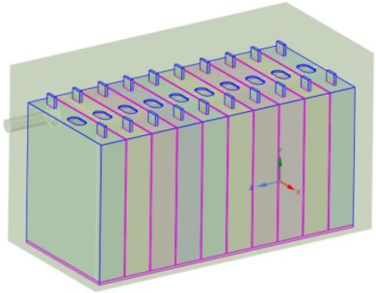
- **Tracing the hot gases** within the battery will **capture a heat transfer mechanism** that is very important in some designs
- **Experimental testing is very expensive** as the prototypes will be destroyed in due process and lab needs special fire protection
- **Gain insight to design heat shields, heat capacities, and flow guides.**

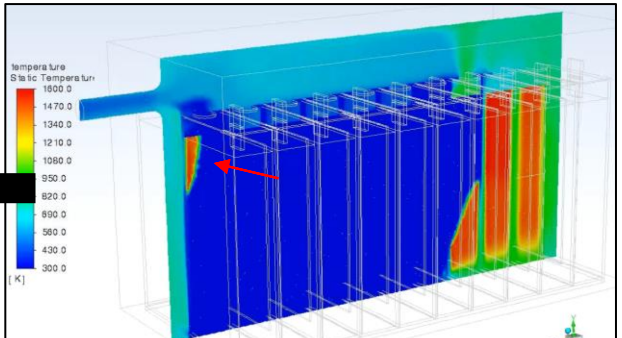


Thermal runaway starts in nail region of cell 1

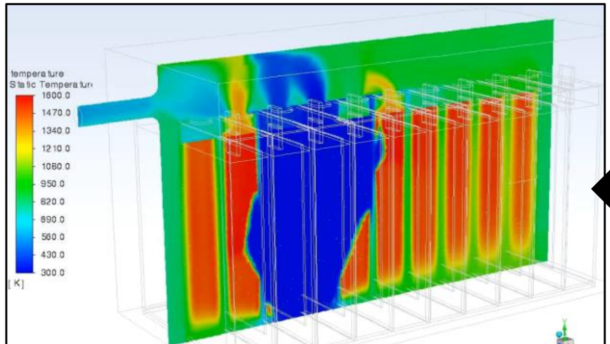


Cell 2 starts by thermal conduction


10 prismatic cells in a module



Cell 10 starts by hot gases



Near the end of thermal runaway

# Appendix

# A thought about experiments

- How good are experiments in reproducing the time to thermal runaway? In the sense of taking 10 new cells of the same kind and bringing them to thermal runaway. What would be the distribution of times measured?