Addressing Challenging Thermal Runaway Simulation Requirements through Detailed 3D CFD Models

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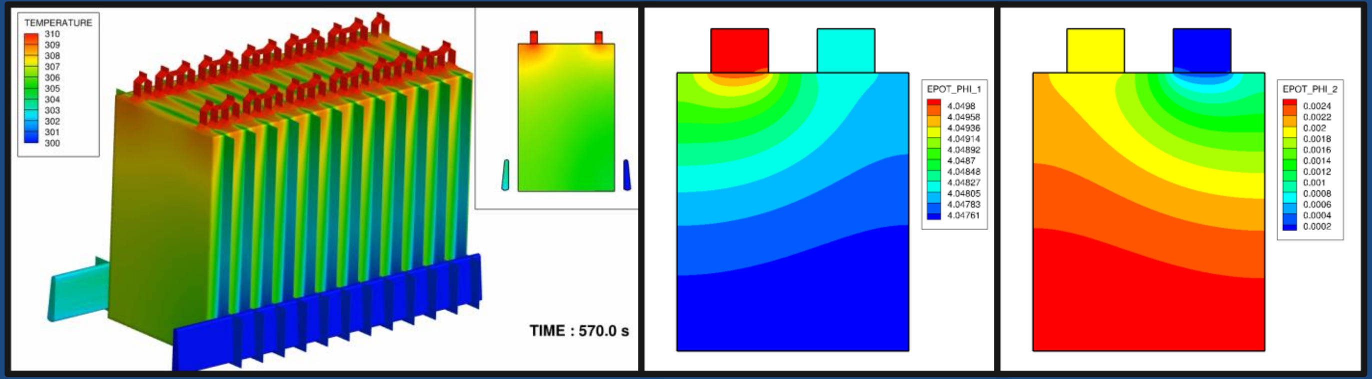
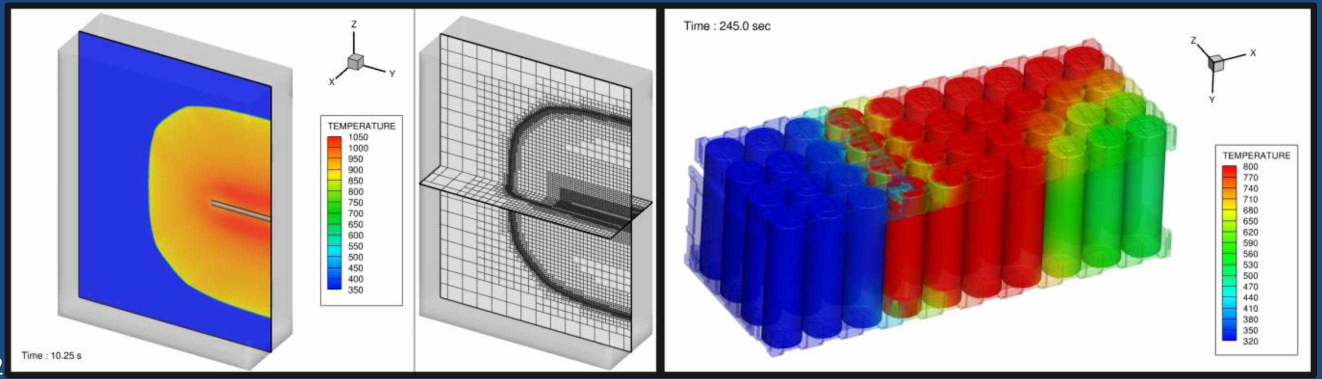
Detailed 3D Battery Simulations Using CONVERGE

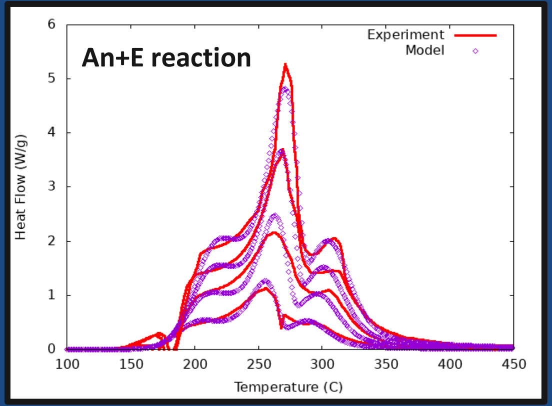
- Air/liquid/immersion cooling, including phase-change materials
  - Electrothermal response using lumped equivalent circuit model or 3D coupled potential solver with electrochemistry

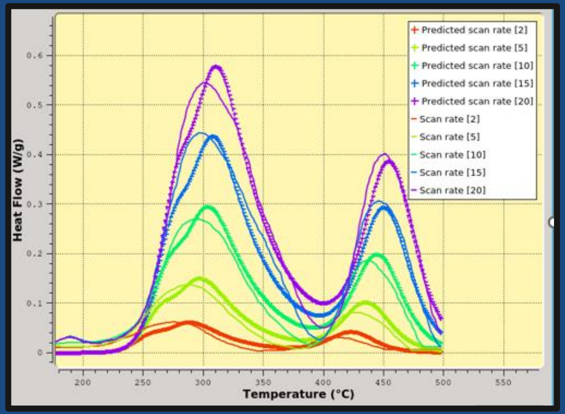


- Thermal runaway propagation: SAGE detailed chemical kinetics solver
  - Arrhenius-based chemical reaction mechanisms

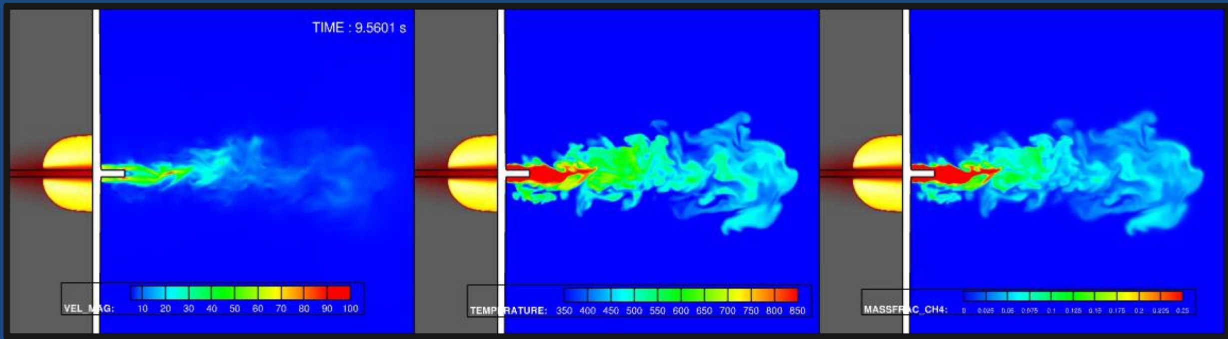


- Thermal runaway mechanism calibration tools
  - ARC Data: Specifying mechanism kinetic parameters
  - DSC Data: Constructing multi-reaction mechanisms

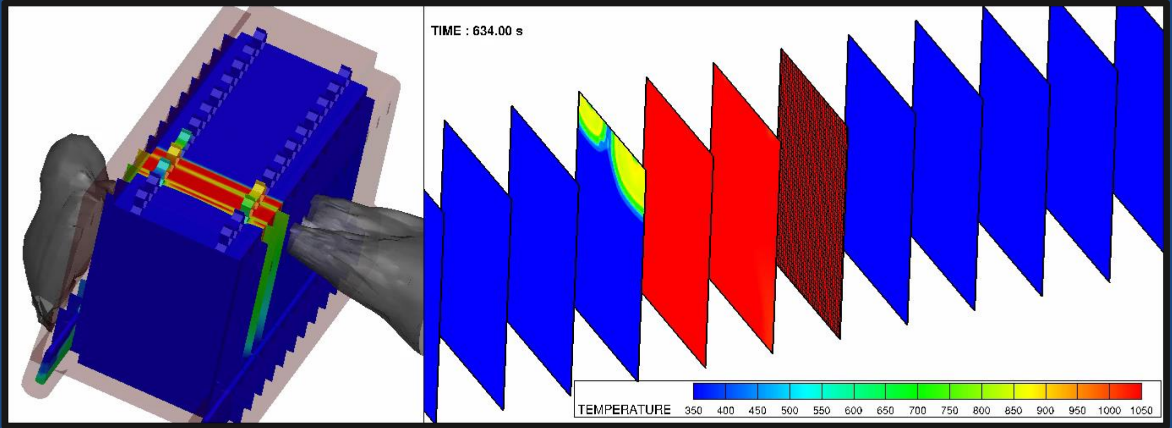




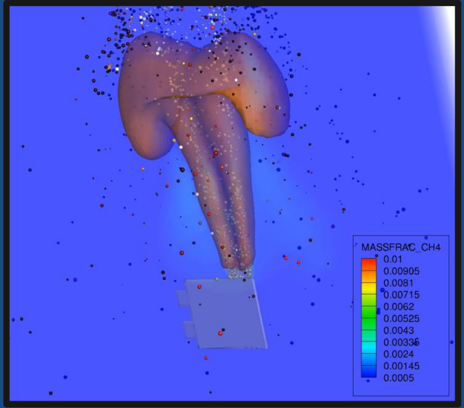
- Thermal runaway vent gas ignition and combustion
  - Vent gas ignition, battery pack fires/explosion, fire suppression, solid ejecta, and deposition



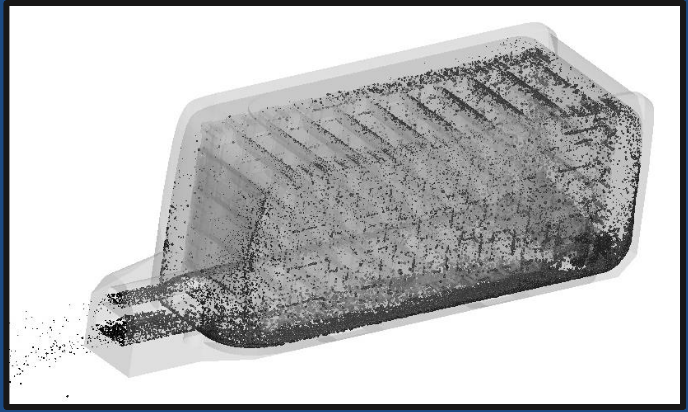
Additional Multi-Physics Simulations Using CONVERGE



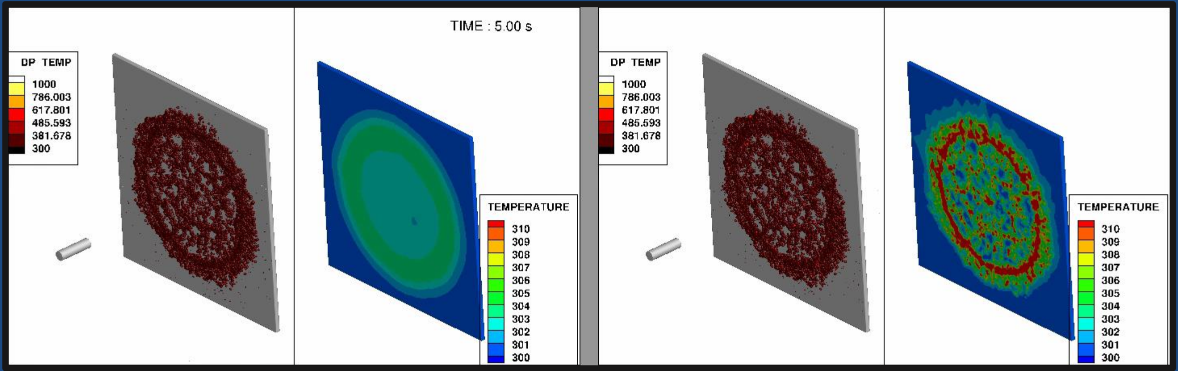
Coupled thermal runaway and venting propagation within a PHEV battery pack module with liquid cold plate cooling (multi-stream simulation)



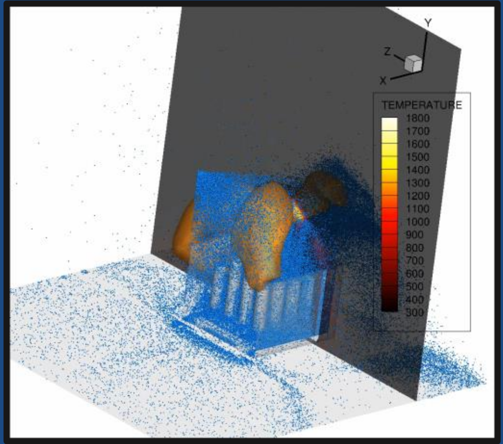
Vent gas ignition due to ejected hot particles



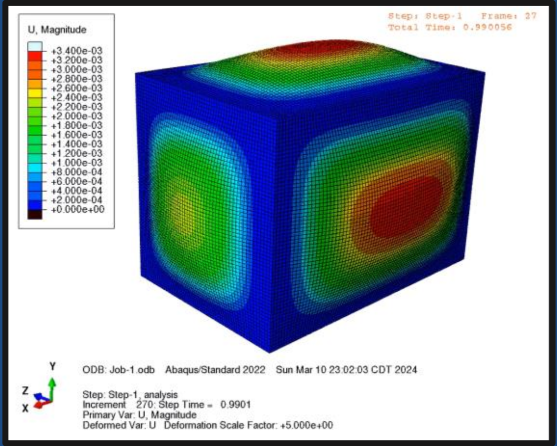
Solid particle ejecta deposition within battery packs



Blast plate heat transfer studies due to solid ejecta during thermal runaway



Battery fire extinguishers



Battery pack swelling (Abaqus coupling)

* Ren, D., Liu, X., Feng, X., Lu, L. Ouyang, M., Li, J., and He, X., *"Model-based thermal runaway prediction of lithium-ion batteries from kinetics analysis of cell components,"* Applied Energy, 228, 633-644, 2018.

Thermal Runaway Mechanisms in CONVERGE

REN TR MECHANISM

- 6 reactions, NMC battery chemistry
  - Ren et al., 2018 *

$$\kappa_x = A_x \cdot \exp\left(-\frac{E_{a,x}}{RT}\right) \cdot f_x(c_x)$$

$$c_x = 1 - \int \kappa_x \, dt$$

$$f_x(c_x) = c_x^{n_x} \qquad Q_x = m_x \cdot \Delta H_x \cdot \kappa_x$$

$$c_{SEI} = 1 - \int \kappa_{SEI} dt$$

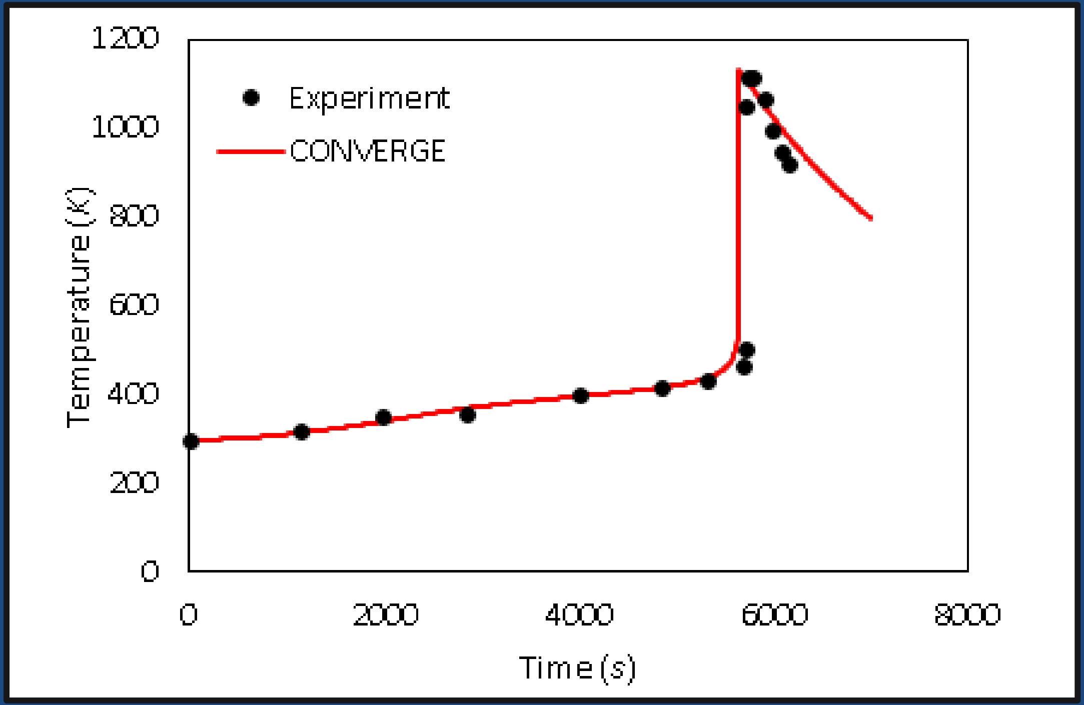
$$c_{An-E} = c_{Cat-An} = 1 - \int (\kappa_{An-E} + \kappa_{Cat-An}) dt$$

$$c_{An-B} = c_{Cat-B} = 1 - \int \left(\frac{\gamma}{1+\gamma} \cdot \kappa_{An-B} + \kappa_{Cat-B}\right) dt$$

$$c_{Cat} = 1 - \int \kappa_{Cat} dt$$

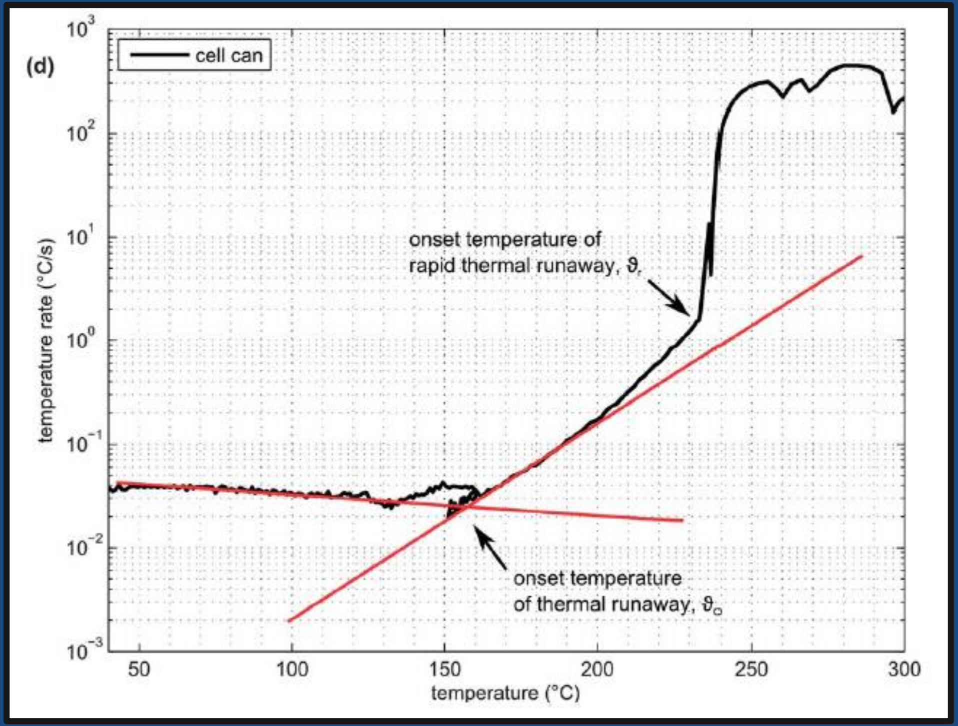
$$Q_{gen} = Q_{SEI} + Q_{An-E} + Q_{An-B} + Q_{Cat-An} + Q_{Cat-B} + Q_{cat}$$

SEI film decomposition (SEI)
Anode and electrolyte (An-E)
Anode and binder (An-B)
Cathode and anode (Cat-An)
Cathode and binder (Cat-B)
Cathode decomposition (Cat)



EV-ARC validation of an NMC pouch cell

Selecting Suitable Thermal Runaway Mechanisms



A.W. Golubkov et. al., "*Thermal-runaway experiments on consumer Li-ion batteries with metal-oxide and olivin-type cathodes*"

$$\kappa_x = A_x \cdot \exp\left(-\frac{E_{a,x}}{RT}\right) \cdot f_x(c_x)$$

$$f_x(c_x) = c_x^{n_x}$$

$$Q_x = m_x \cdot \Delta H_x \cdot \kappa_x$$

Fighting Thermal Runaway Propagation

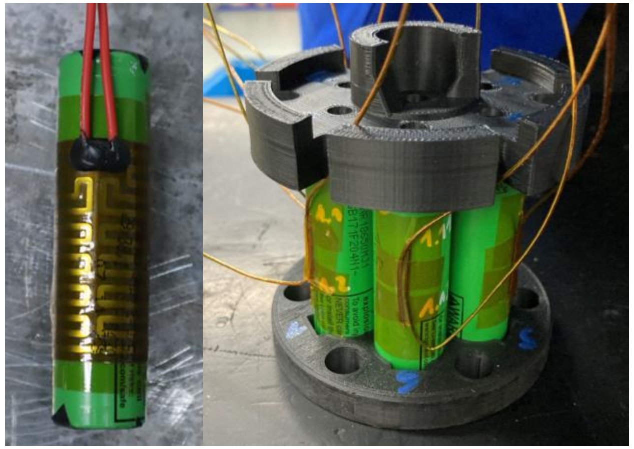
- Collaborative work between IAV GmbH and Convergent Science Inc.
- Addressing the ever-increasing risk for Thermal Runaway Propagation
    - Evaluation across different development targets : Cell chemistry, Cell format, Cell2Battery configuration, Thermal management, Venting system
- Assess mitigation technologies and develop novel methodologies
- Thermal management operation strategy optimization : Predictive 3D simulation approaches
- Work published at the 45th International Vienna Motor Symposium

Sens, M., Fandakov, A., Mueller, K., von Roemer, L., Woebke, M., Tourlonias, P., Mueller, T., Burton, T., Srivastava, K., and Senecal, P.K., “**From Thermal Runaway to No Thermal Propagation**,” *45th International Vienna Motor Symposium*, Vienna, Austria, Apr 24–26, 2024. https://doi.org/10.62626/wznd-tsm7

The Path to No Thermal Runaway Propagation

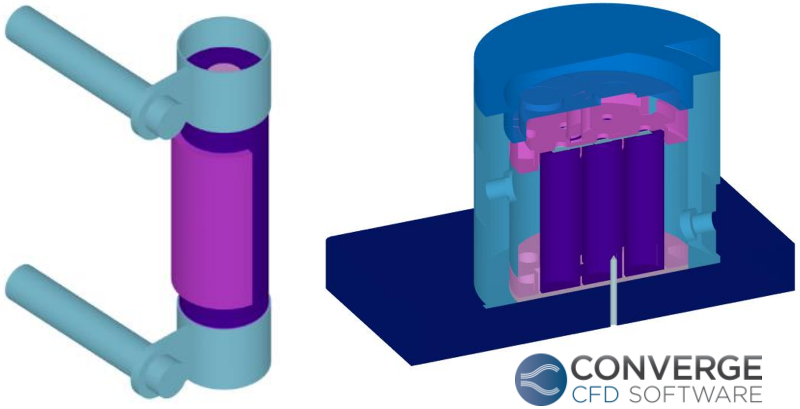
Extensive single cell and cell assembly testing within IAV test facilities

- Different cell chemistries, cell assembly set-ups, TR initiation methods, propagation mitigation measures
- Measurement data to help validate TR and TRP simulation approaches
- Understanding TRP process at critical conditions with different mitigation technologies



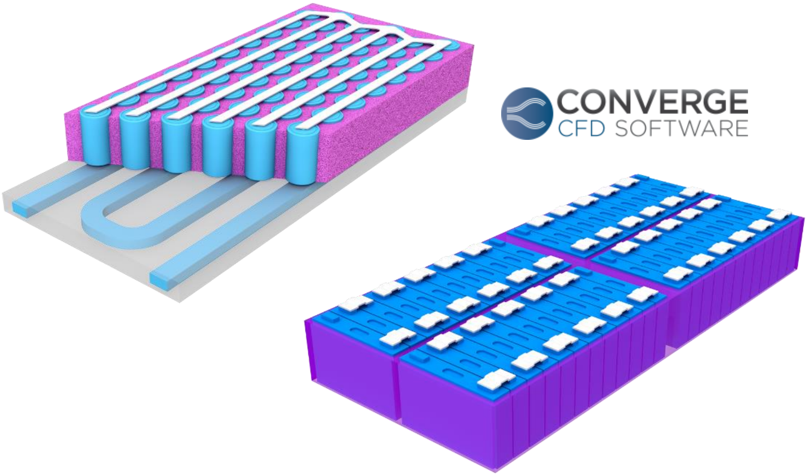
Simulation methodology development and validation using CONVERGE

- Chemistry-based TR mechanism calibration for different cell chemistries
- Validation with single cell characterizations
- Transfer to cell assembly models and validation with assembly measurements
- Consideration of thermal management, pack configuration, vent gases, gas combustion

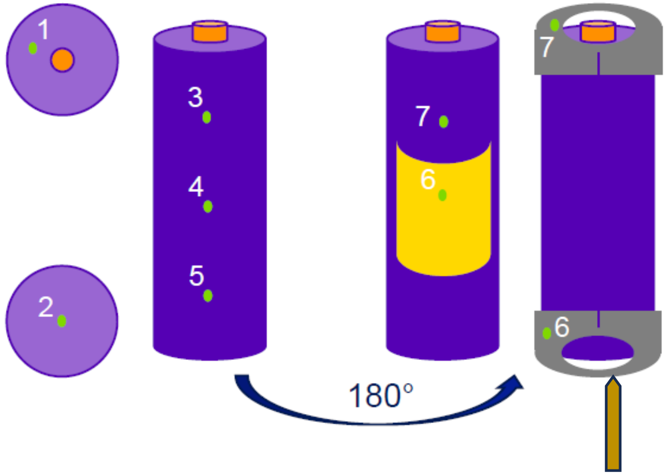


Investigation of new TRP mitigation technologies through detailed 3D CFD

- Deployment of validated TR mechanisms and cell assembly models
- Virtual assessment of different technologies for slowing down or mitigating TRP : Foams, compression pads, oil, PCMs, etc.



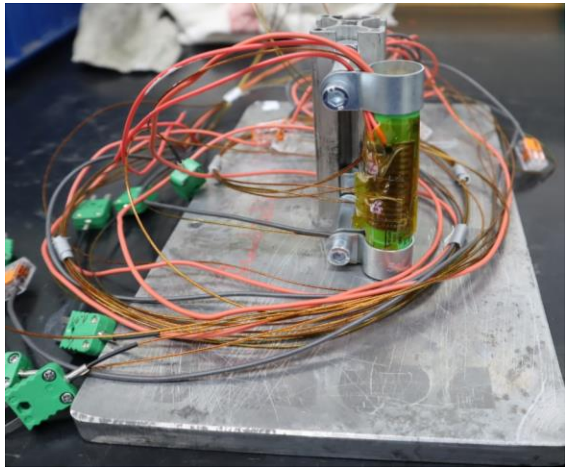
Single Cell Testing

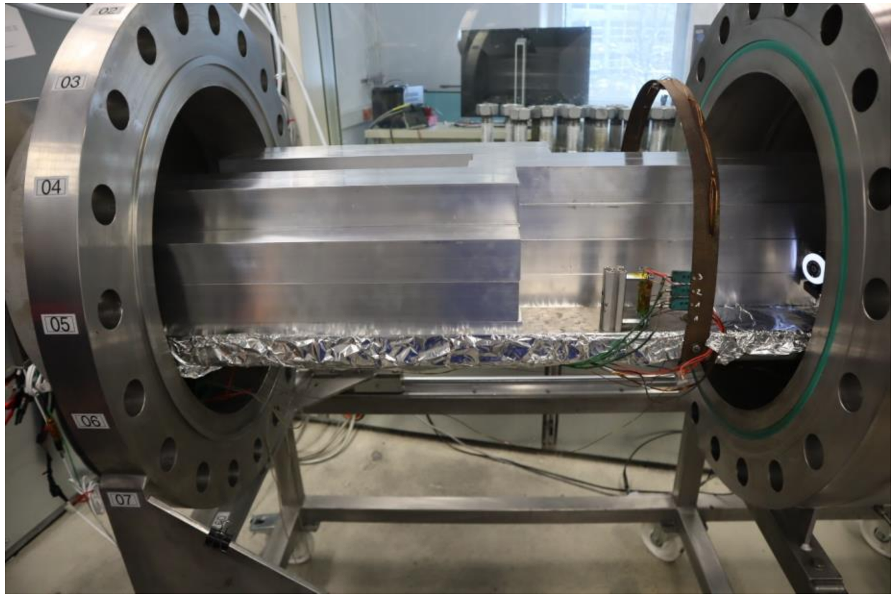


TC	HWS / CH test	NP test
1	cell top, next to center	
2	cell bottom, centered	
3	side at 1/4 height	
4	side at 1/2 height	
5	side at 3/4 height	
6	on heating pad	on bottom holder
7	above heating pad	on top holder

Heating pad (Heat-wait-seek / Constant heating)

Cell holder (Nail penetration)

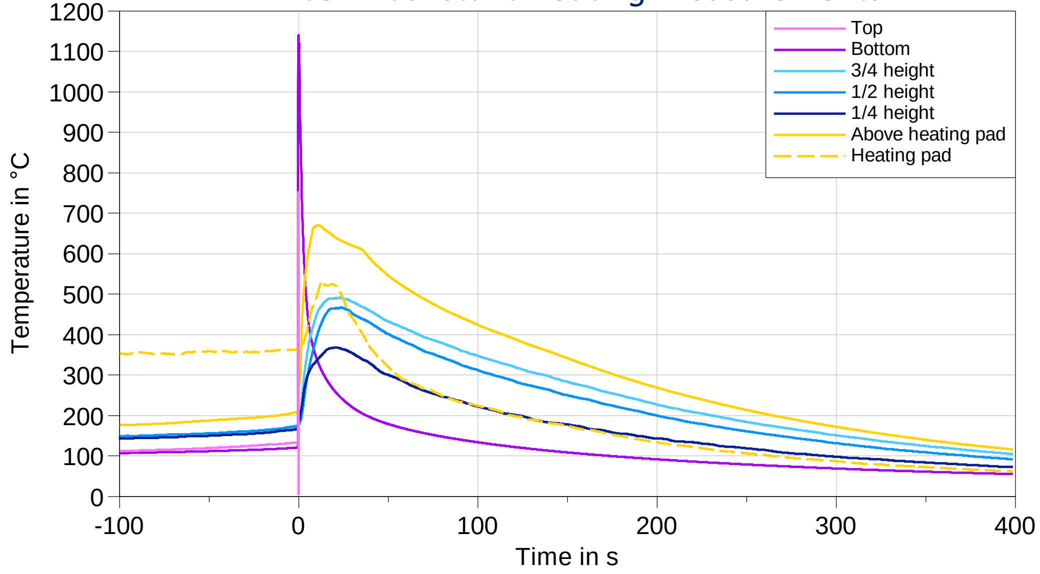


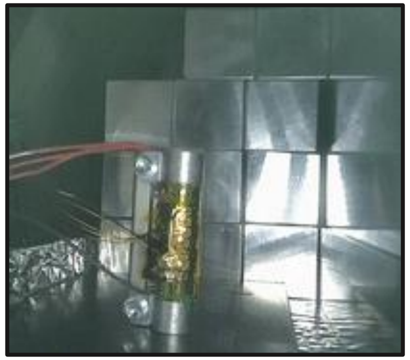


- Cell chemistry and triggering method comparison
  - NMC811, LFP, SIB : 18650 Cylindrical format
  - Constant heating (CH), Heat-Wait-Seek(HWS), Nail Penetration
- Cell tests conducted by IAV in an autoclave under an inert (N_2) atmosphere

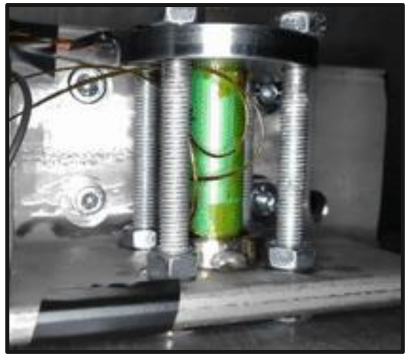
Single Cell Testing : Results

NMC811 Constant Heating Measurements



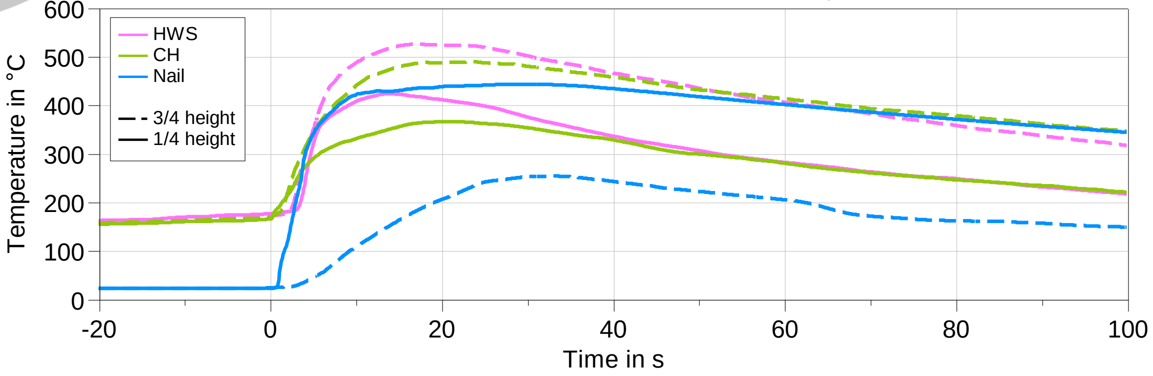


NMC811 CH

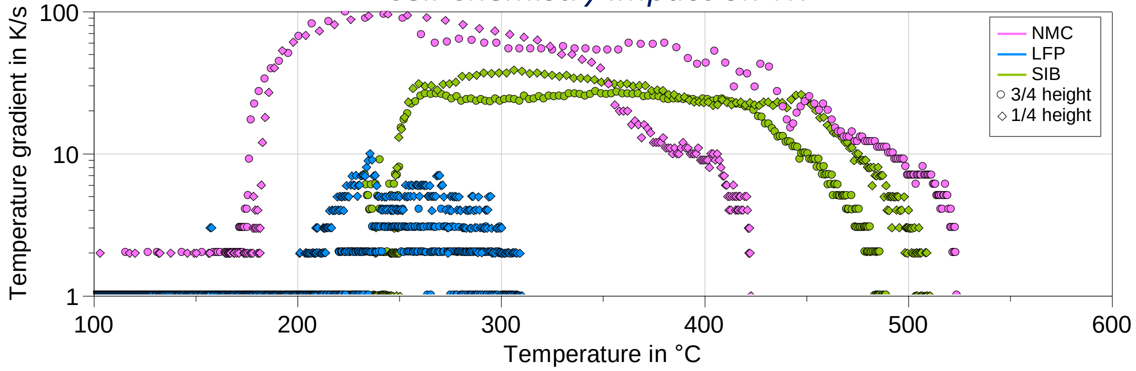


NMC811 Nail

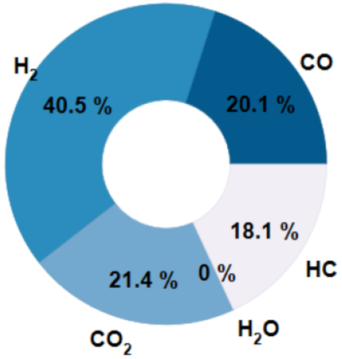
NMC811 TR Initiation Method Impact



Cell Chemistry Impact on TR

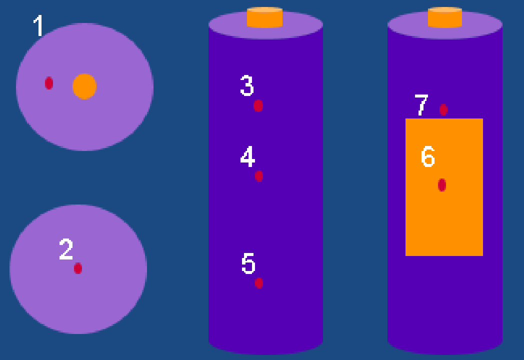


NMC811 Gas Analysis

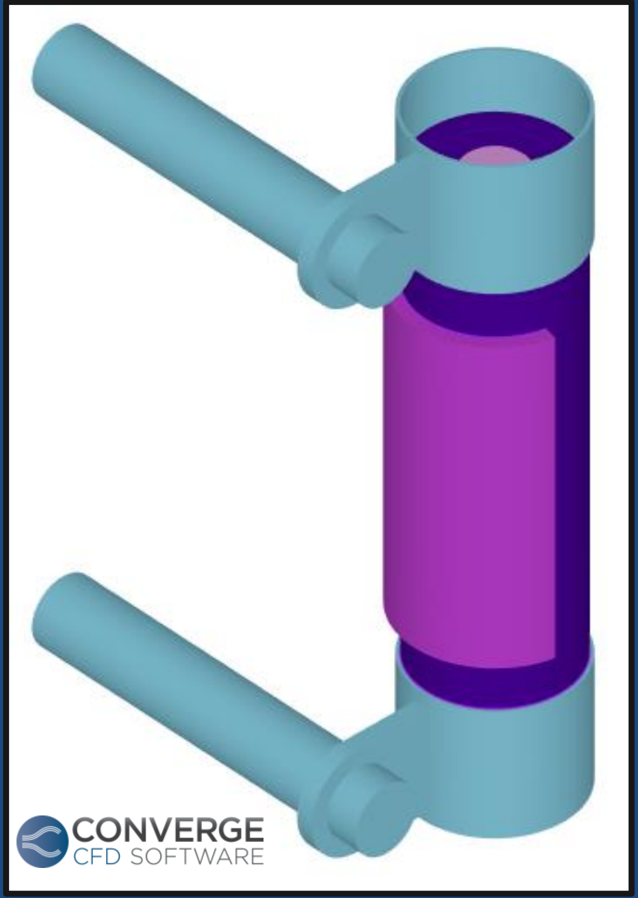


CO	20.0577
H_2	40.4724
CO_2	21.3665
H_2O	0
HC	18.1033

Ethyne	0.509592
Propene	2.69707
Propane	1.82094
Ethene	9.68279
Ethane	1.63644
Butadiene	1.74261
Methane	18.9755
Methanol	8.11549
DMC	55.3152
EMC	0.71025

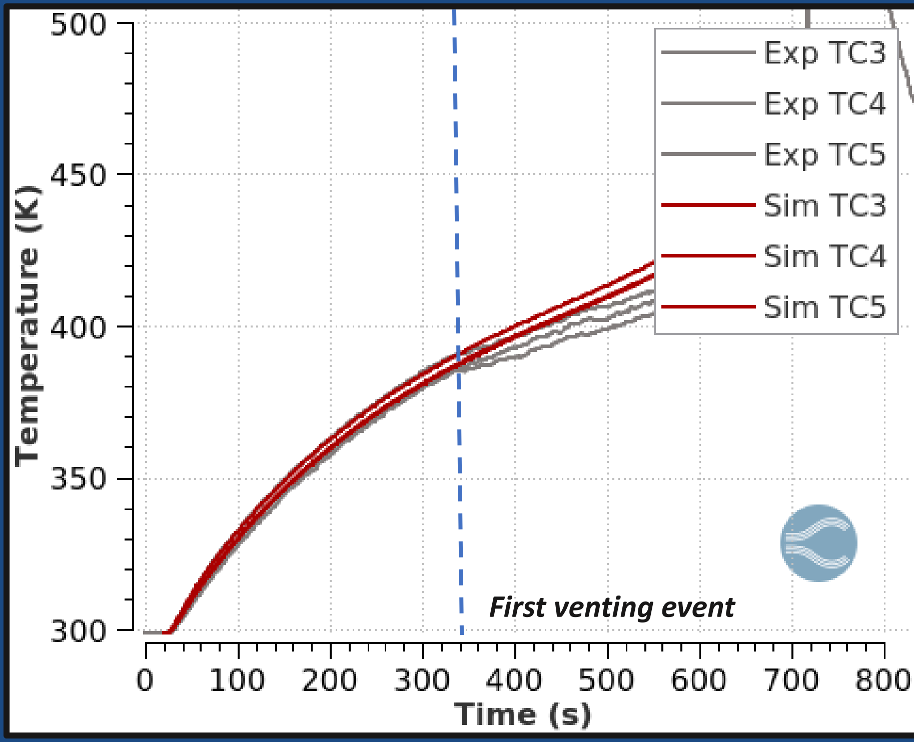


Single Cell Calibration Setup



- NMC811 constant heating experiment chosen for REN mechanism calibration
- Thermocouples 3, 4, 5 selected as reliable for calibration process

- Solid-only CONVERGE 3D simulation
- Thermal properties included
  - 18650 NMC811 cell
  - Heating pad
  - Clamps
- Solid-solid CHT interfaces between parts
- Outer walls: Convection temperature BC
  - Heat loss to surroundings
  - HTC calibrated to match initial battery warm-up behavior
- First venting observed around 340 *s*

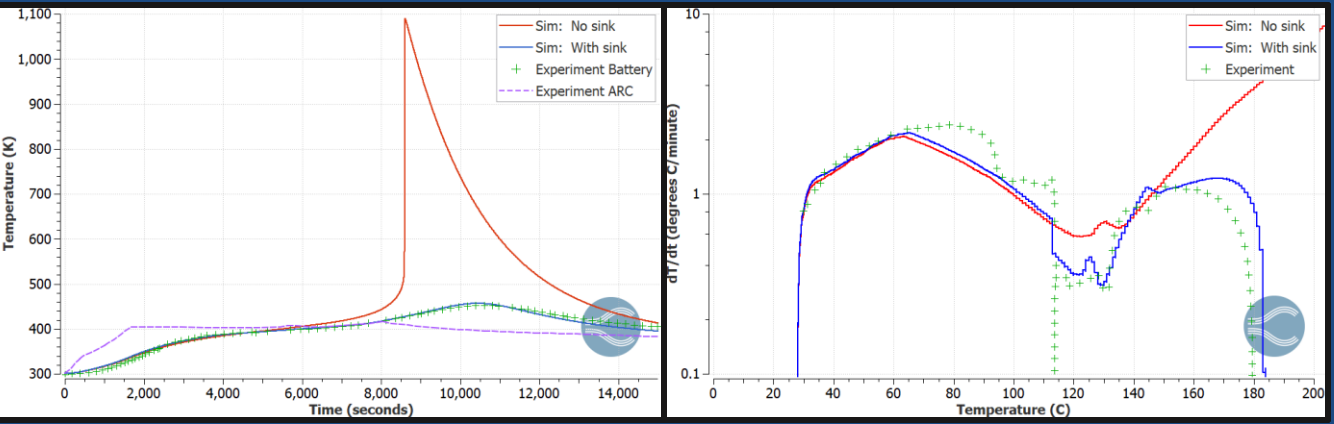


Calibrated HTC = 29 W/m^{2}K

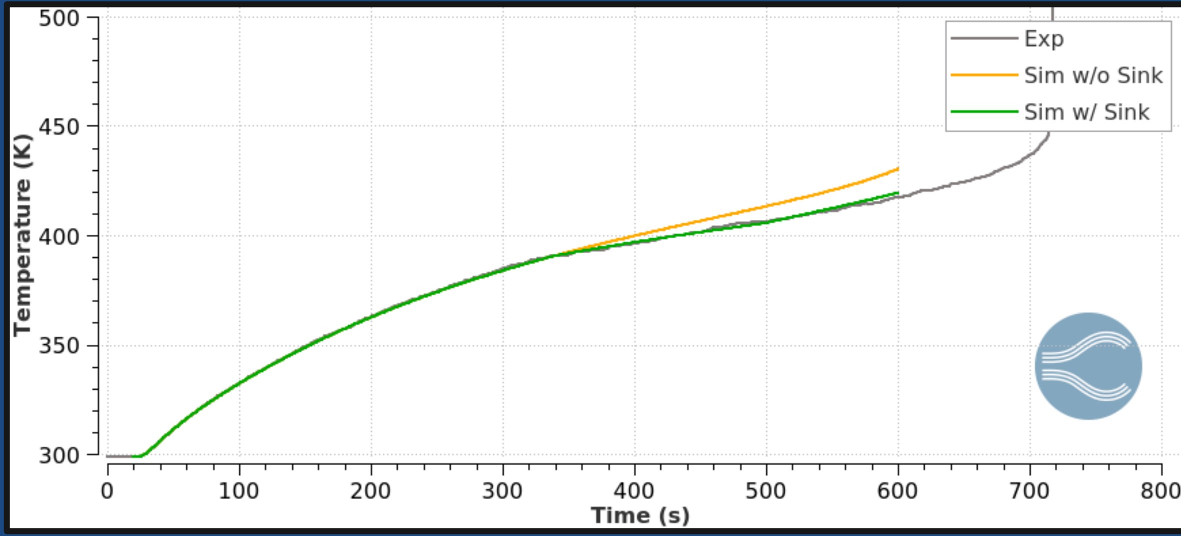
* Ostanek, J.K., Li, W., Mukherjee, P.P., Crompton, K.R., and Hacker, C., *"Simulating onset and evolution of thermal runaway in Li-ion cells using a coupled thermal and venting model,"* Applied Energy, 268, 114972, 2020
+ Parhizi, M., Crompton, K., and Ostanek, J., *"Probing the Role of Venting and Evaporative Cooling in Thermal Runaway for Small Format Li-Ion Cells."*, ASME International Mechanical Engineering Congress and Exposition, 2021

Evaporative Cooling

- 130 *°C* Ren et al. case
  - Vaporization of the electrolyte is endothermic (not in the mechanism)
    - 91 *°C* dimethyl carbonate (DMC)
    - 110 *°C* ethyl methyl carbonate (EMC)
    - 248 *°C* ethylene carbonate (EC)
  - Use an energy sink to account for vaporization

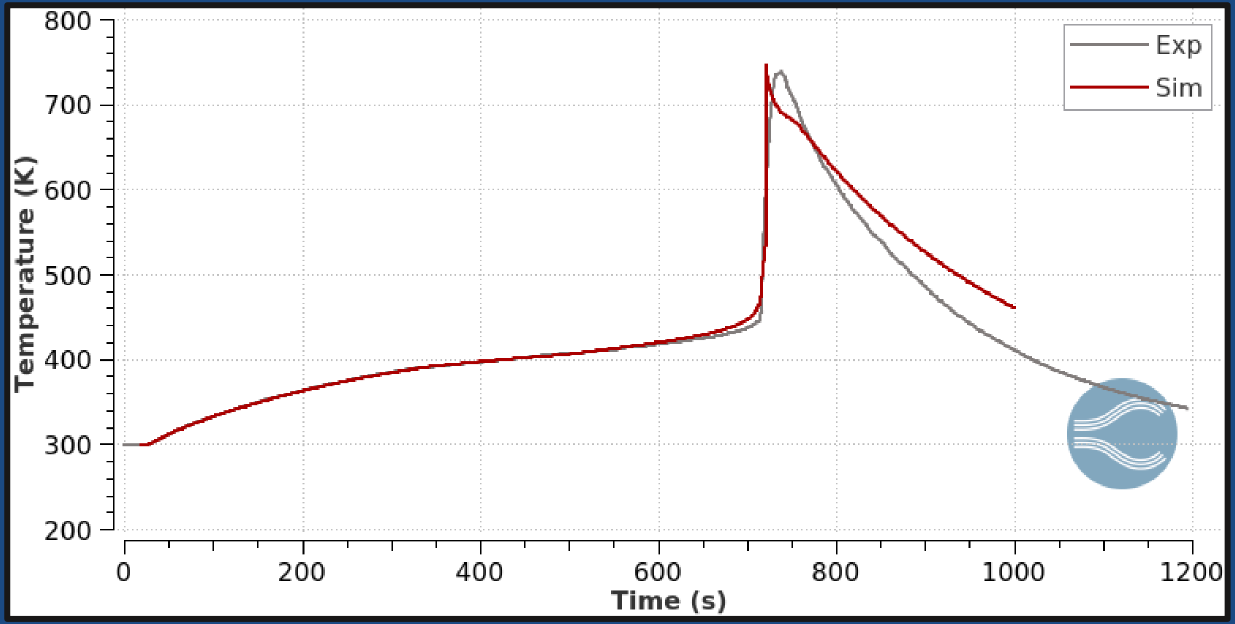


- Evaporative cooling: Heat sink activated at experimentally observed first venting event (~340 *s*)

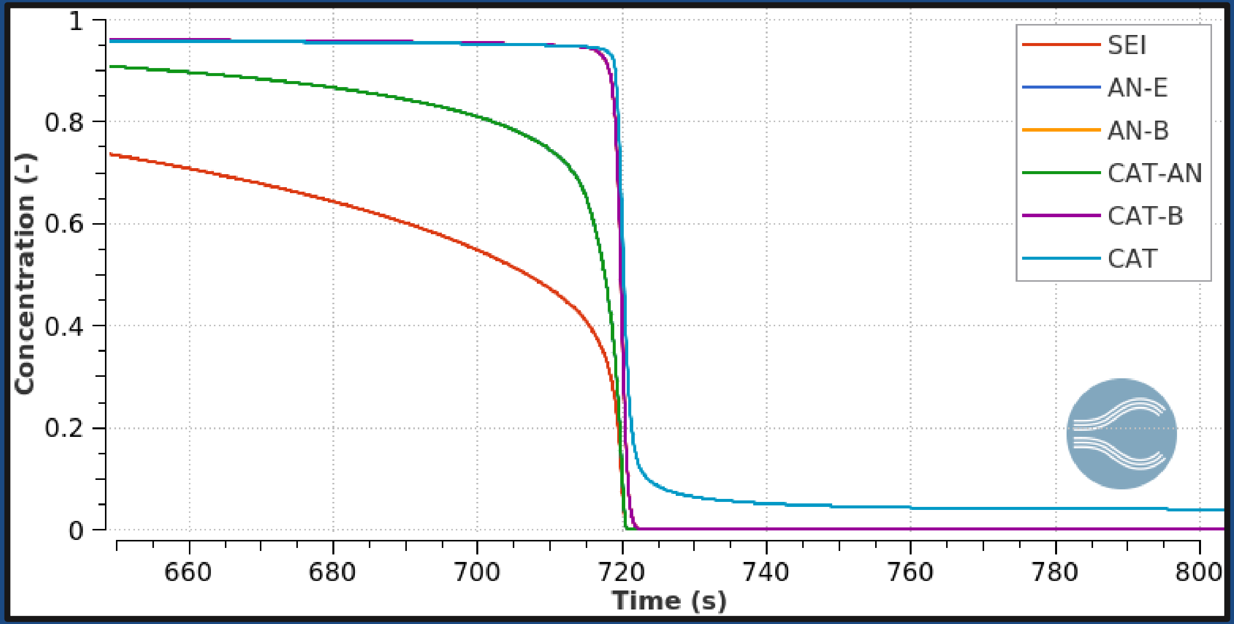


- Calibrated energy sink in agreement with literature
  - Total energy sink applied : -450 *J*
  - Mass of free electrolyte in 18650 : ~ 0.5-1.2 *g* (*Ostanek et al., +Parhizi et al.)
  - Heat of vaporization of electrolyte : -418 *J/g* (+Parhizi et al.,)

REN Mechanism Calibration

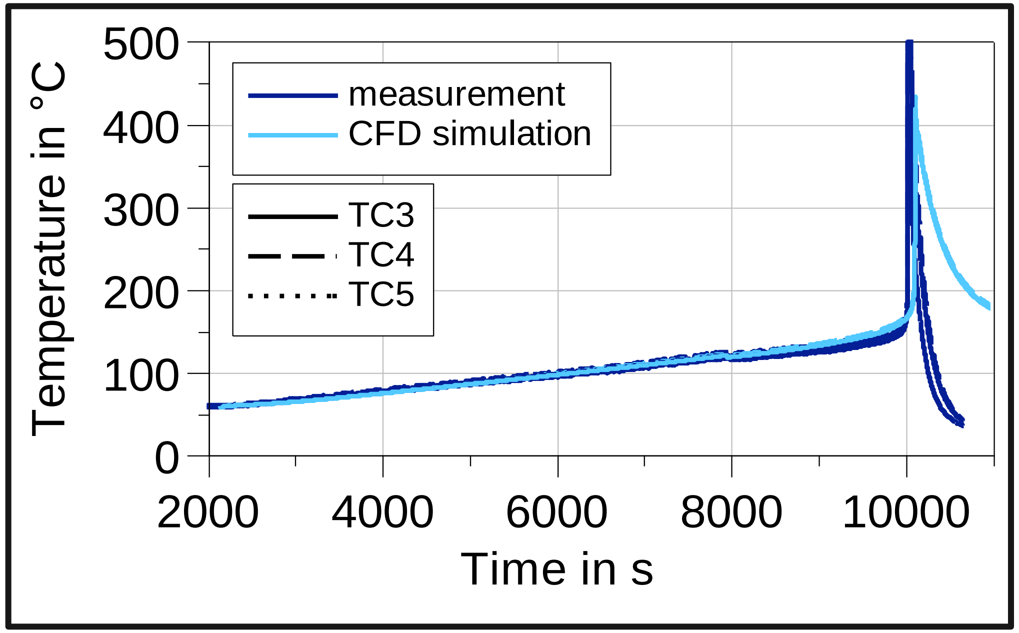


Calibrated REN TR Mechanism

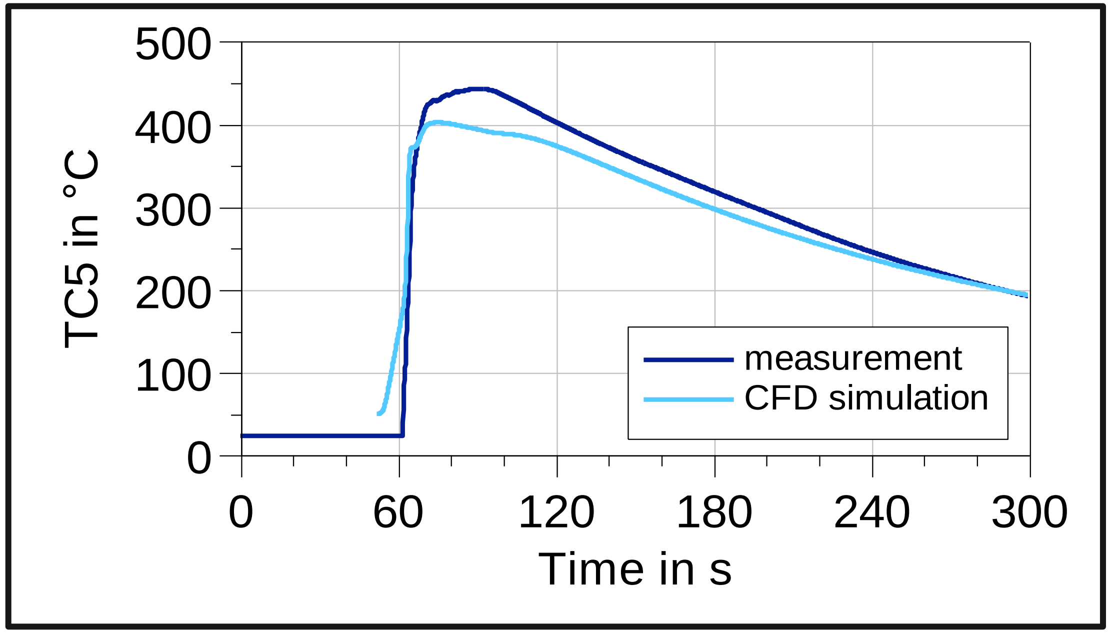


Expected reaction order: SEI → An-E/Cat-An → An-B/Cat-B → Cat

Calibrated REN Mechanism Validation



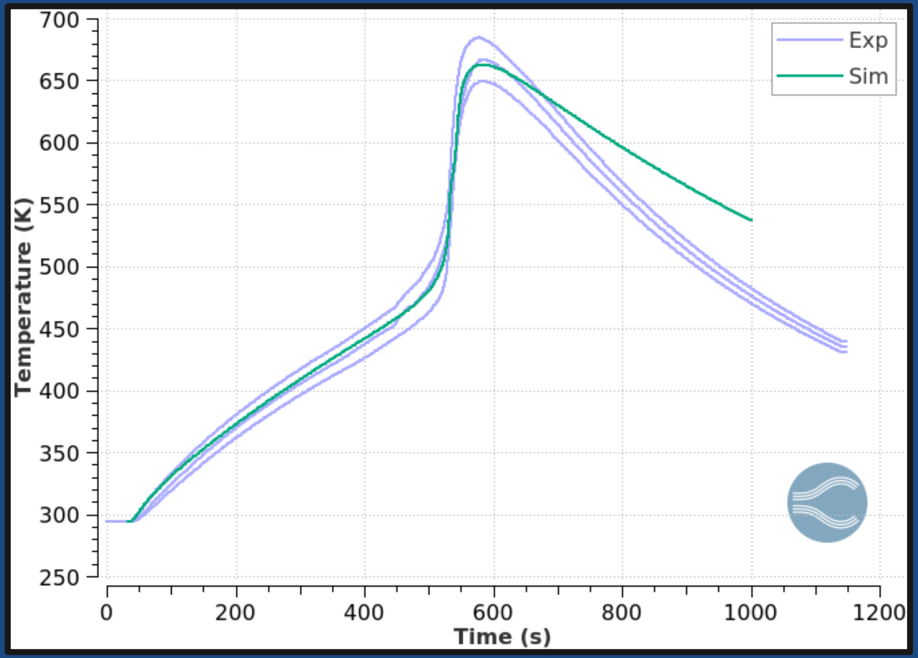
Heat-Wait-Seek



Nail Penetration

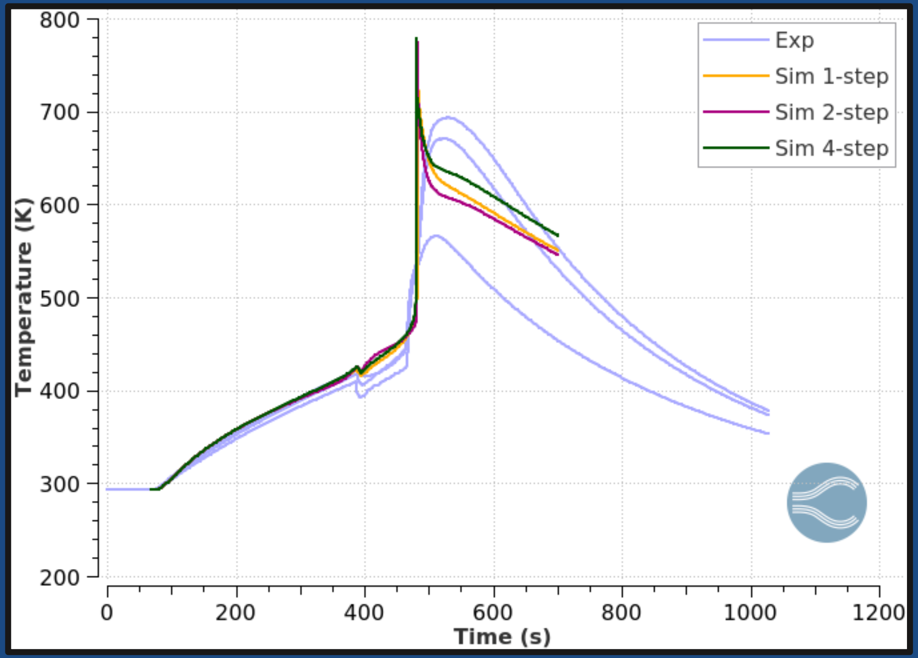
Alternative Battery Chemistries: LFP/SIB

Lithium Iron Phosphate (LFP) Chemistry



Calibrated Hatchard-Kim TR mechanism

Sodium-Ion Battery (SIB)



Calibrated multi-step TR mechanisms

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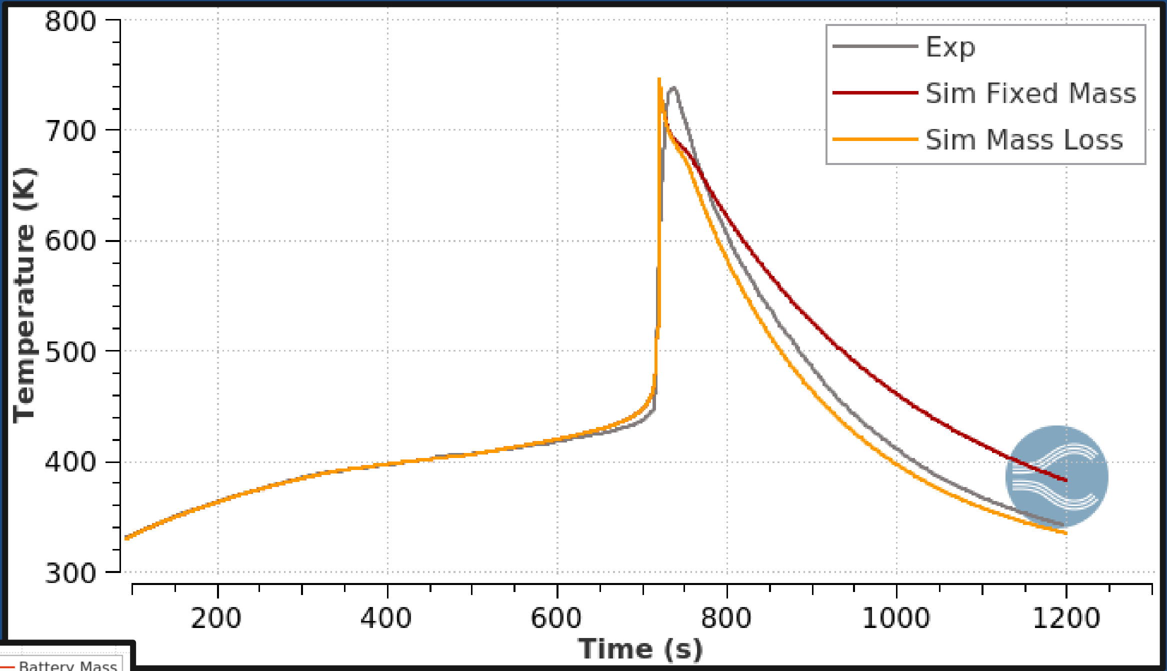
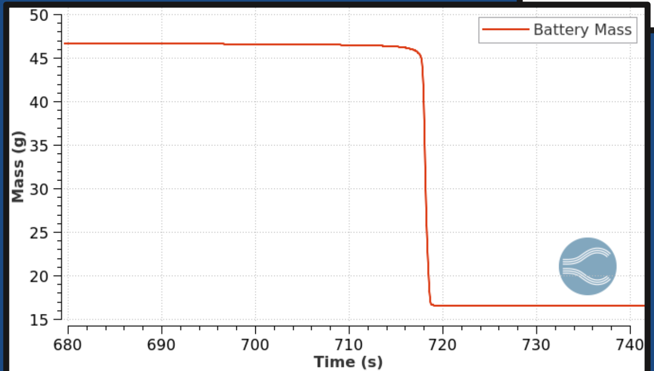
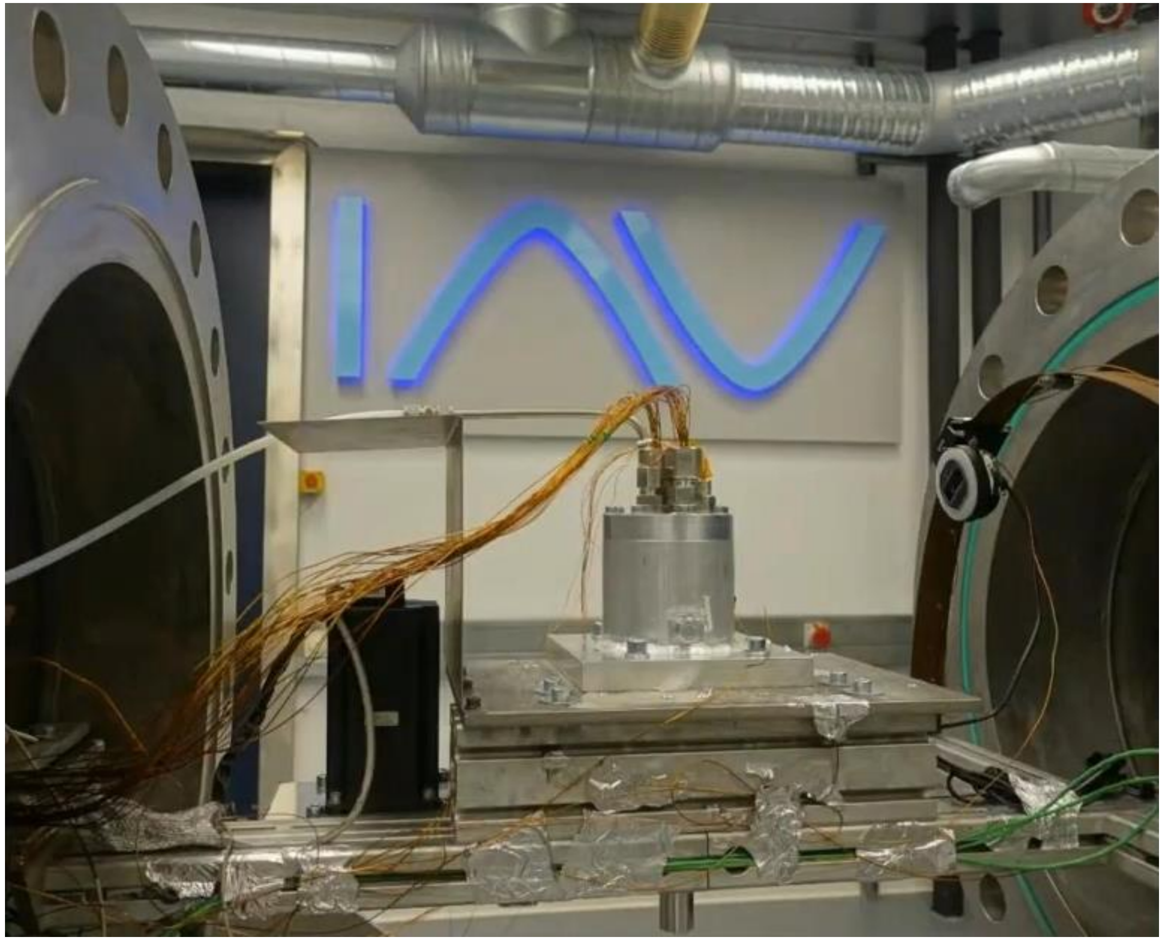
Further Improvement: Mass Loss during TR

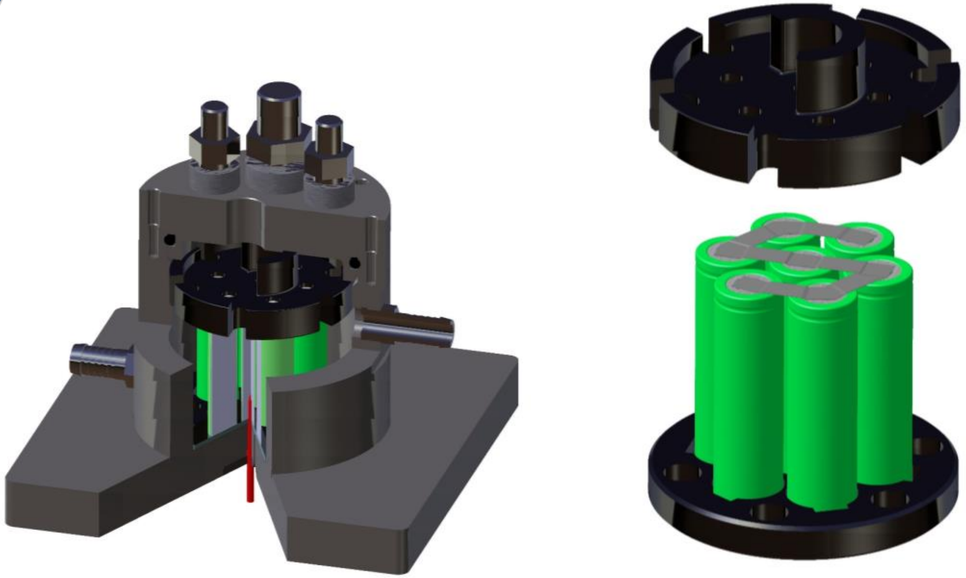
- 64.7% cell weight loss
  - Mainly solid ejecta
- Effect on battery cooldown after TR event
- Dynamic reduction of battery thermal mass ($\rho.C_p$)
  - Coupled to An-B, Cat-B, and Cat decomposition (late-stage) reactions

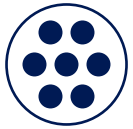


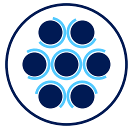


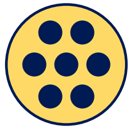
TRP Cell Assembly Testing






Inter-cell Distance


Inter-cell Element (Insulating Foam)

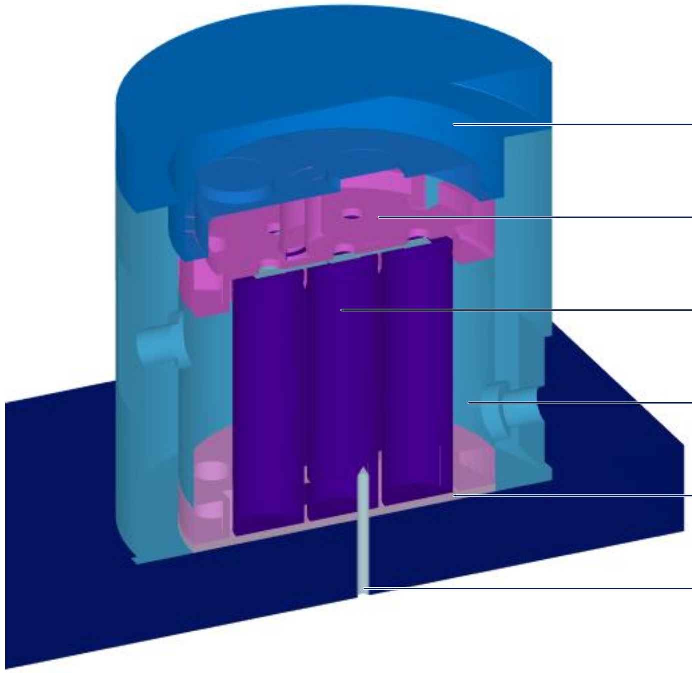

Immersion Oil Setup

- Extensive experimental campaign with 7-Cell module assembly focusing on
    - Understanding TRP process at critical conditions with different mitigation technologies to slow down or stop propagation
    - Generation of measurement data for validating TRP simulation approaches
- TR trigger : Nail penetration of the center cell

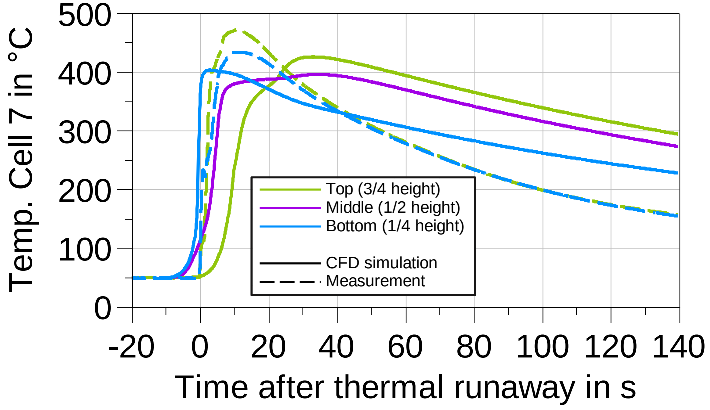
IAV

TRP Model Validation

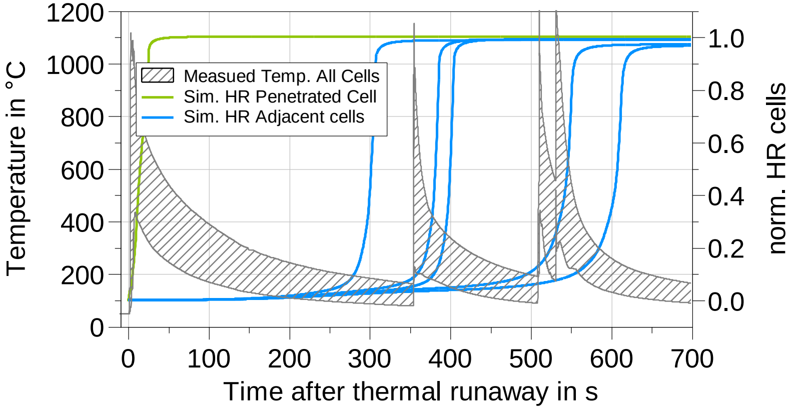
- NMC811 TRP simulations with validated TR mechanism
- Dedicated modeling simplifications applicable for balancing between accuracy and computation effort (ex. Gas reactions, oil boiling)
- Good representation of TRP characteristics and overall test results
- Max. TRP duration error ~10%, equal number of TR events



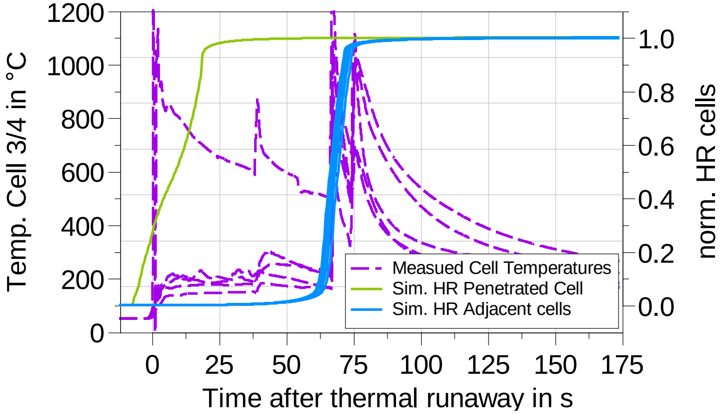
50 °C | N_2
TR behaviour in trigger cell



50 °C | N_2
Inter-cell element

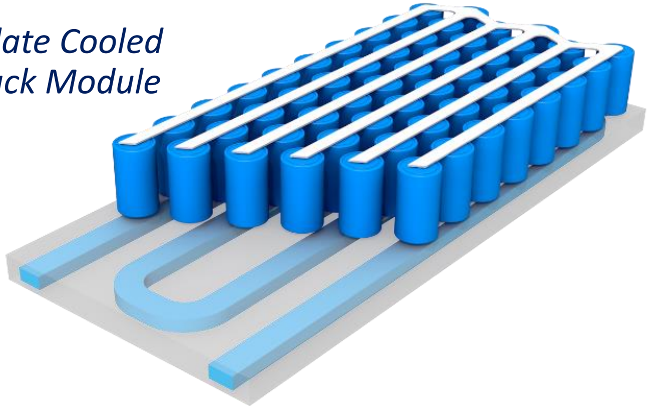


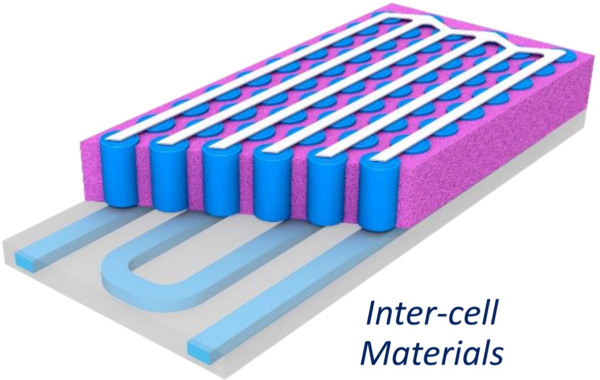
50 °C | Oil
Dielectric fluid w/o flow



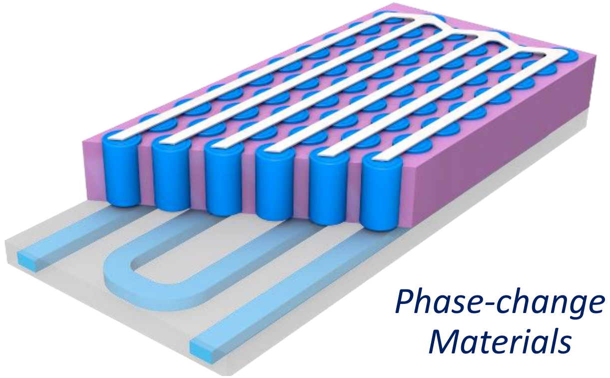
Path Towards No Propagation : Designing Safer Packs

Air + Liquid Plate Cooled EV Battery Pack Module

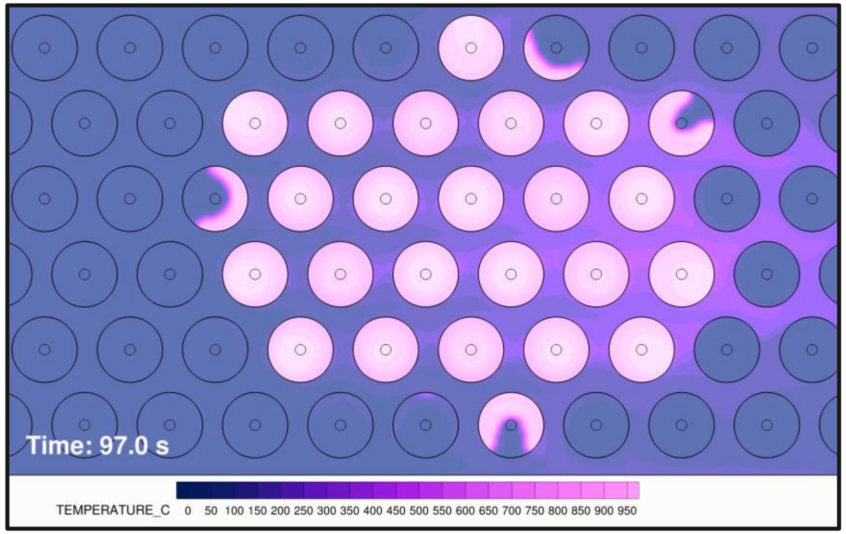


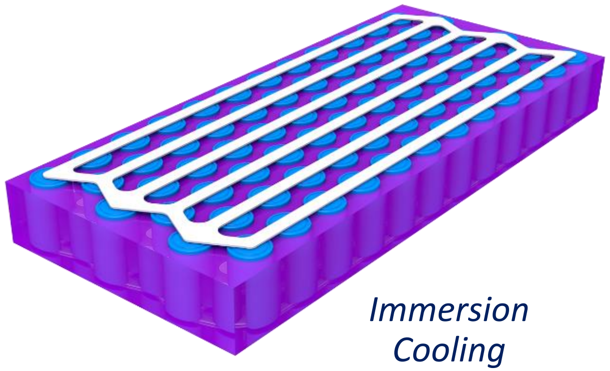


Inter-cell Materials

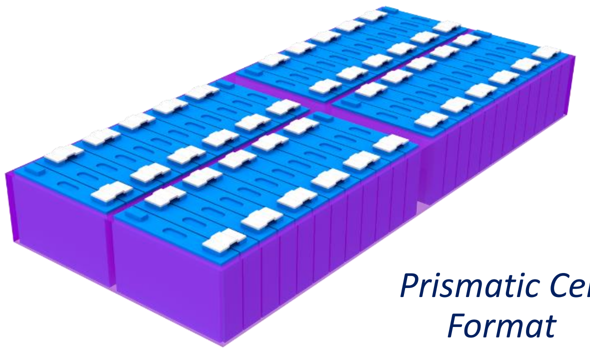


Phase-change Materials





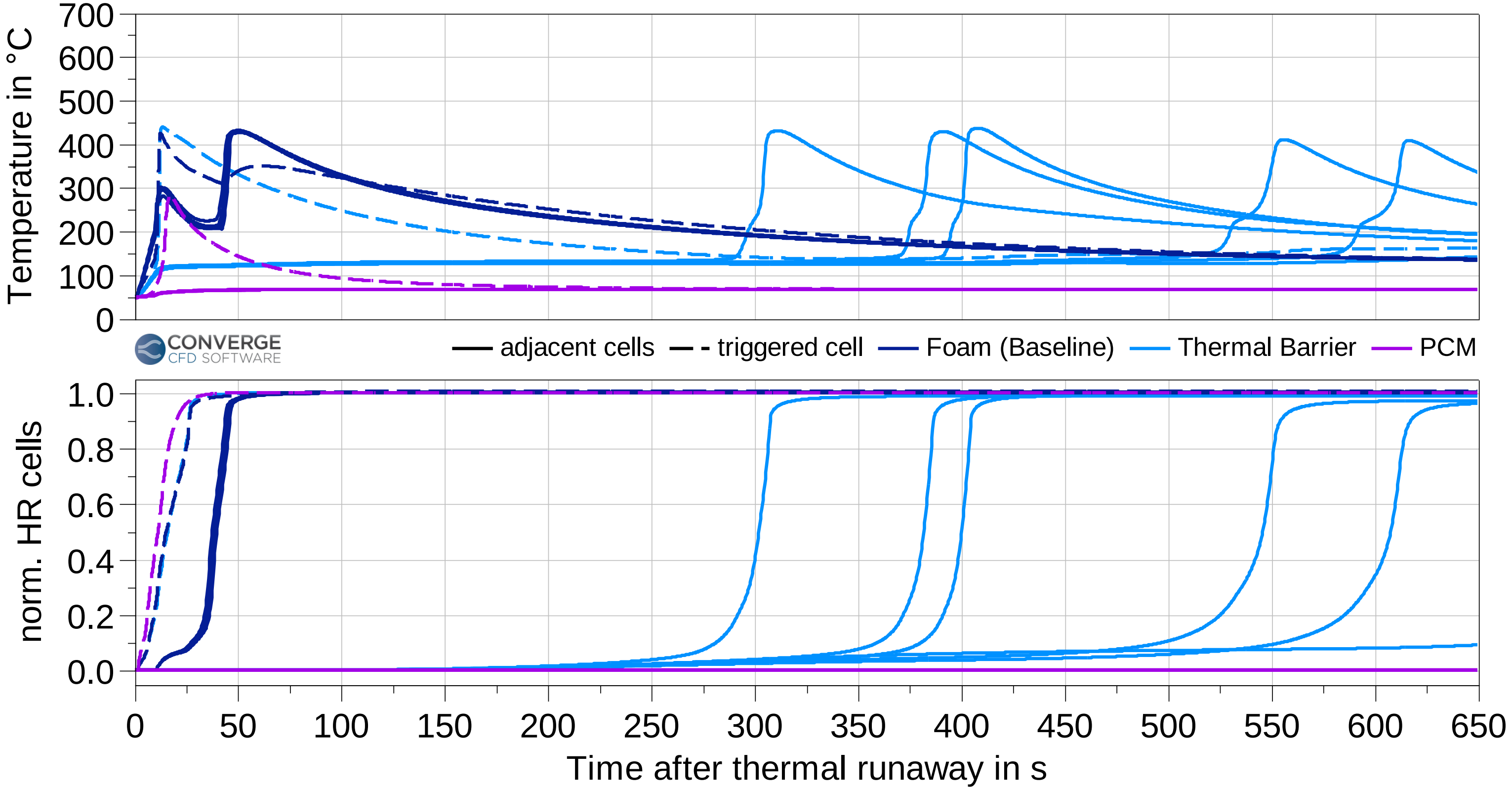
Immersion Cooling



Prismatic Cell Format

IAV

Cylindrical Cell EV Module : Inter-Cell Material



Properties of Technical Solution

Foam

Conductivity	Reference
Density	Reference
Cp	Reference

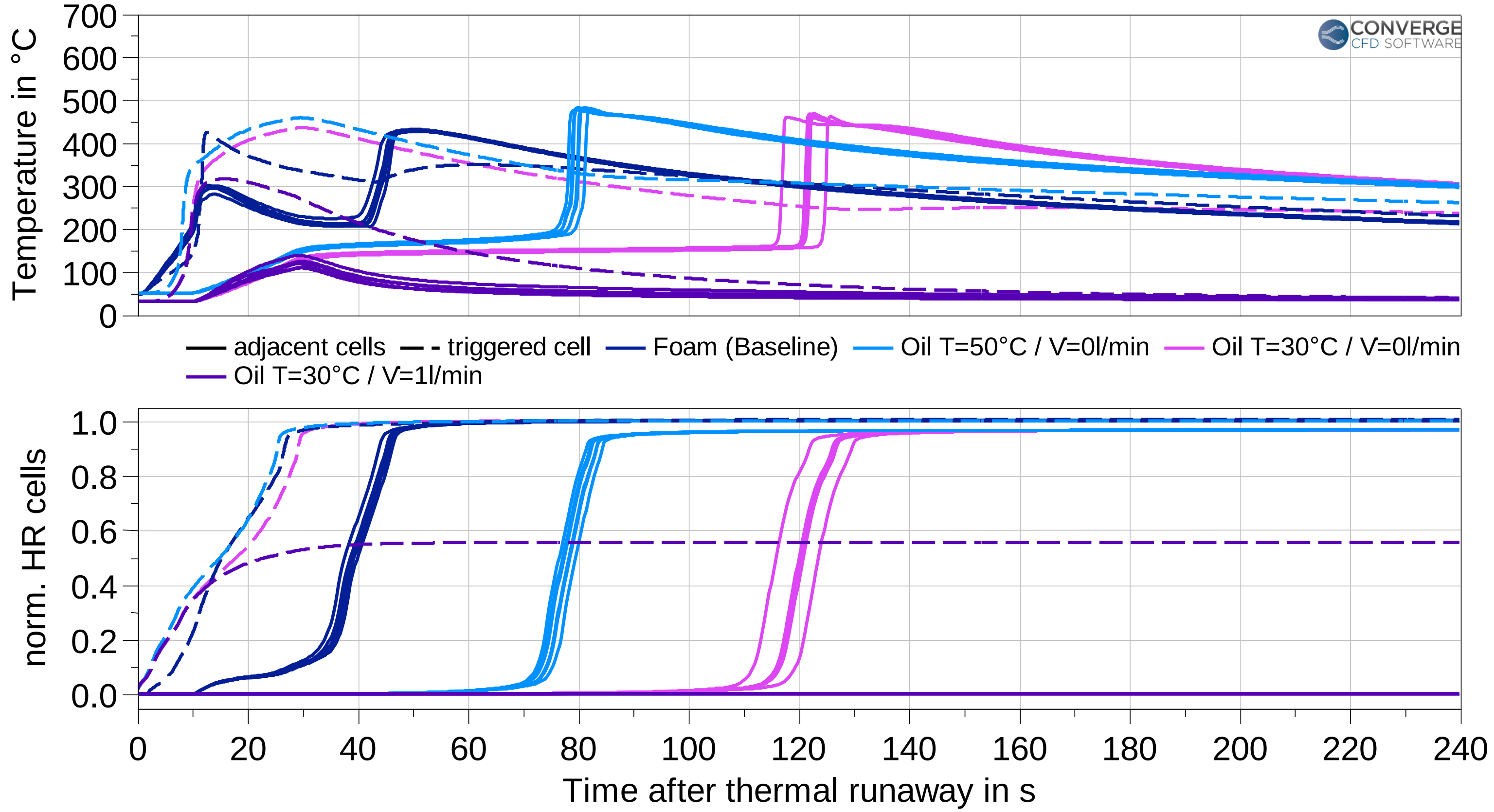
Thermal Barrier

Conductivity	↘↘↘
Density	↘↘
Cp	→

PCM

Conductivity	↘
Density	↘
Cp	↗

Cylindrical Cell EV Module : Immersion Cooling

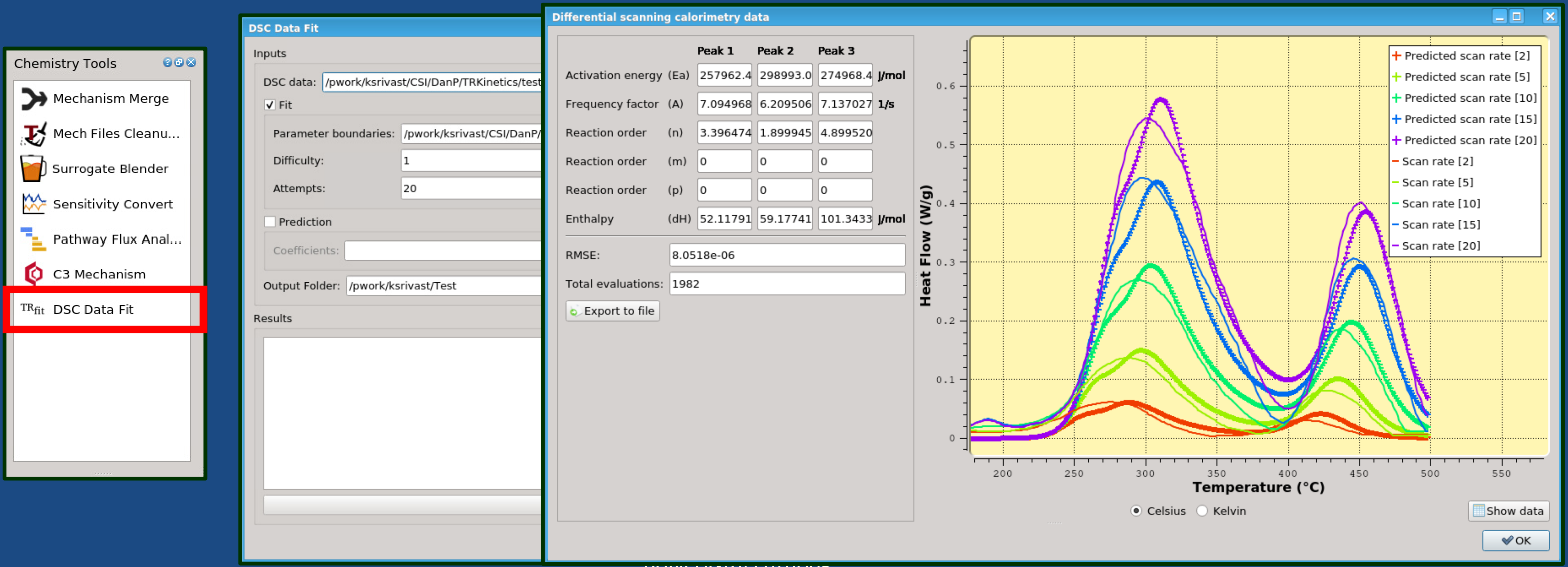


Properties of Technical Solution

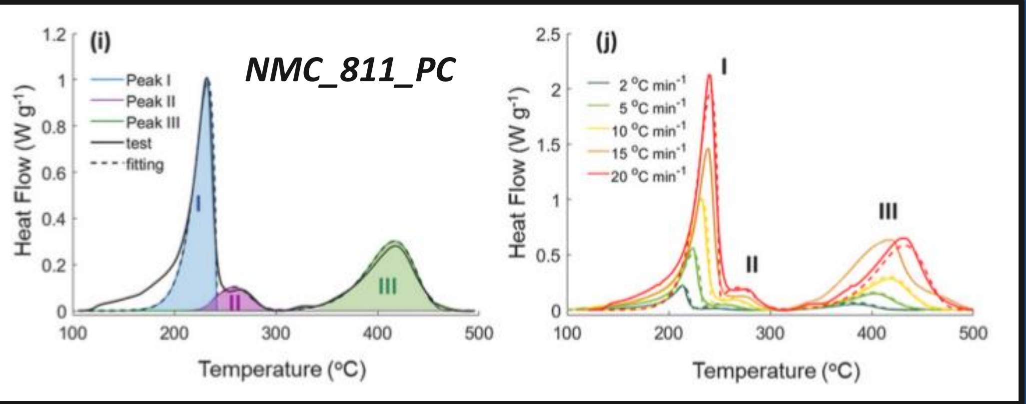
Foam	
Conductivity	Reference
Density	Reference
Cp	Reference
Oil w/o flow at 50 °C	
Conductivity	↘↘
Density	↘
Cp	↗
Oil w/o flow at 30 °C	
Conductivity	↘↘
Density	↘
Cp	↗
Oil flow at 30 °C	
Conductivity	↘↘
Density	↘
Cp	↗

TR Mechanism Generation/Fitting: DSC Data Fit Tool

- Generate/fit TR reaction parameters based on provided reaction format and parameter bounds

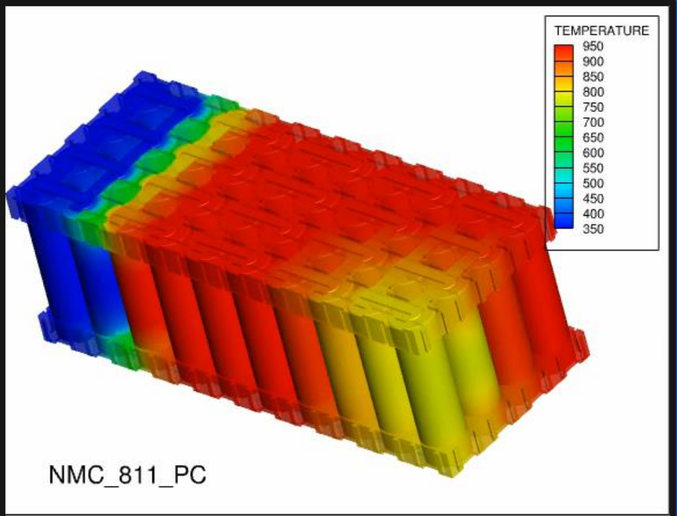


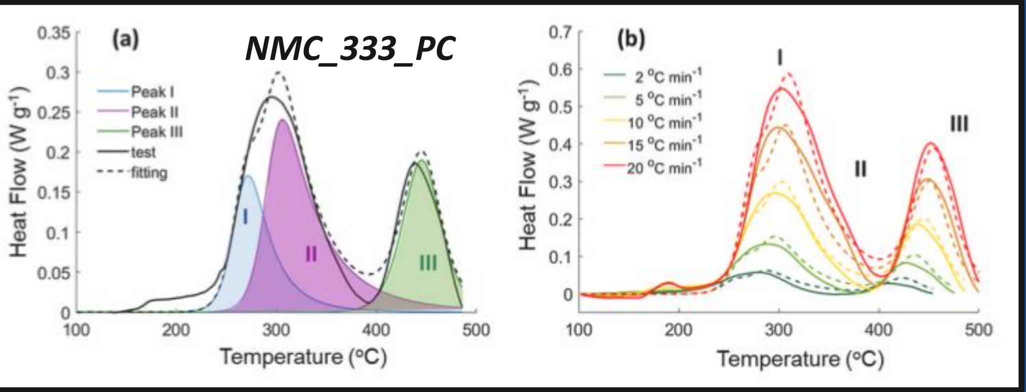
NMC Cathode Composition: Effect on TR Propagation



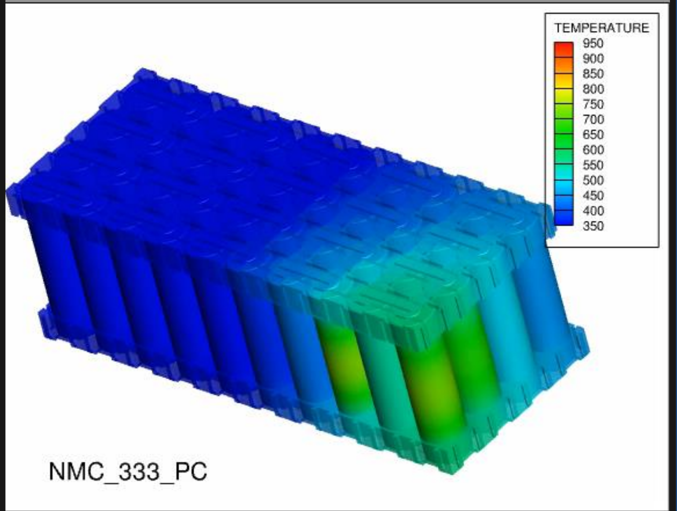
Wang, Yu et.al., *Thermal kinetics comparison of delithiated Li[Ni Co Mn]O2 cathodes*. Journal of Power Sources, 2021

```
## Cathode reaction inputs :  Wang2021
# reaction1
2.80E15          Acat1                 # Frequency factor (1/s)
1.68E5           Ecat1                 # Activation energy (J/mol)
145000           Hcat1                 # Reaction enthalpy (J/kg)
0.6              ncat1                 # Reaction order (-)
1.0              ccat10                # Initial concentration (-)
# reaction2
5.50E13          Acat2                 # Frequency factor (1/s)
1.60E5           Ecat2                 # Activation energy (J/mol)
24000            Hcat2                 # Reaction enthalpy (J/kg)
1.3              ncat2                 # Reaction order (-)
1.0              ccat20                # Initial concentration (-)
# reaction3
4.70E10          Acat3                 # Frequency factor (1/s)
1.69E5           Ecat3                 # Activation energy (J/mol)
109000           Hcat3                 # Reaction enthalpy (J/kg)
1.0              ncat3                 # Reaction order (-)
1.0              ccat30                # Initial concentration (-)
# cathode content
512.48           mcat                  # Specific content (kg/m^3)
```






```
## Cathode reaction inputs :  Wang2021
# reaction1
7.10E22          Acat1                 # Frequency factor (1/s)
2.58E5           Ecat1                 # Activation energy (J/mol)
52000            Hcat1                  # Reaction enthalpy (J/kg)
3.4              ncat1                  # Reaction order (-)
1.0              ccat10                 # Initial concentration (-)
# reaction2
7.10E22          Acat2                  # Frequency factor (1/s)
2.75E5           Ecat2                  # Activation energy (J/mol)
101000           Hcat2                  # Reaction enthalpy (J/kg)
4.9              ncat2                  # Reaction order (-)
1.0              ccat20                 # Initial concentration (-)
# reaction3
6.20E19          Acat3                  # Frequency factor (1/s)
2.99E5           Ecat3                  # Activation energy (J/mol)
59000            Hcat3                  # Reaction enthalpy (J/kg)
1.9              ncat3                  # Reaction order (-)
1.0              ccat30                 # Initial concentration (-)
# cathode content
512.48           mcat                  # Specific content (kg/m^3)
```



Species-based TR Mechanisms

Chemical Thermal Runaway Modeling of Lithium-Ion Batteries for Prediction of Heat and Gas Generation

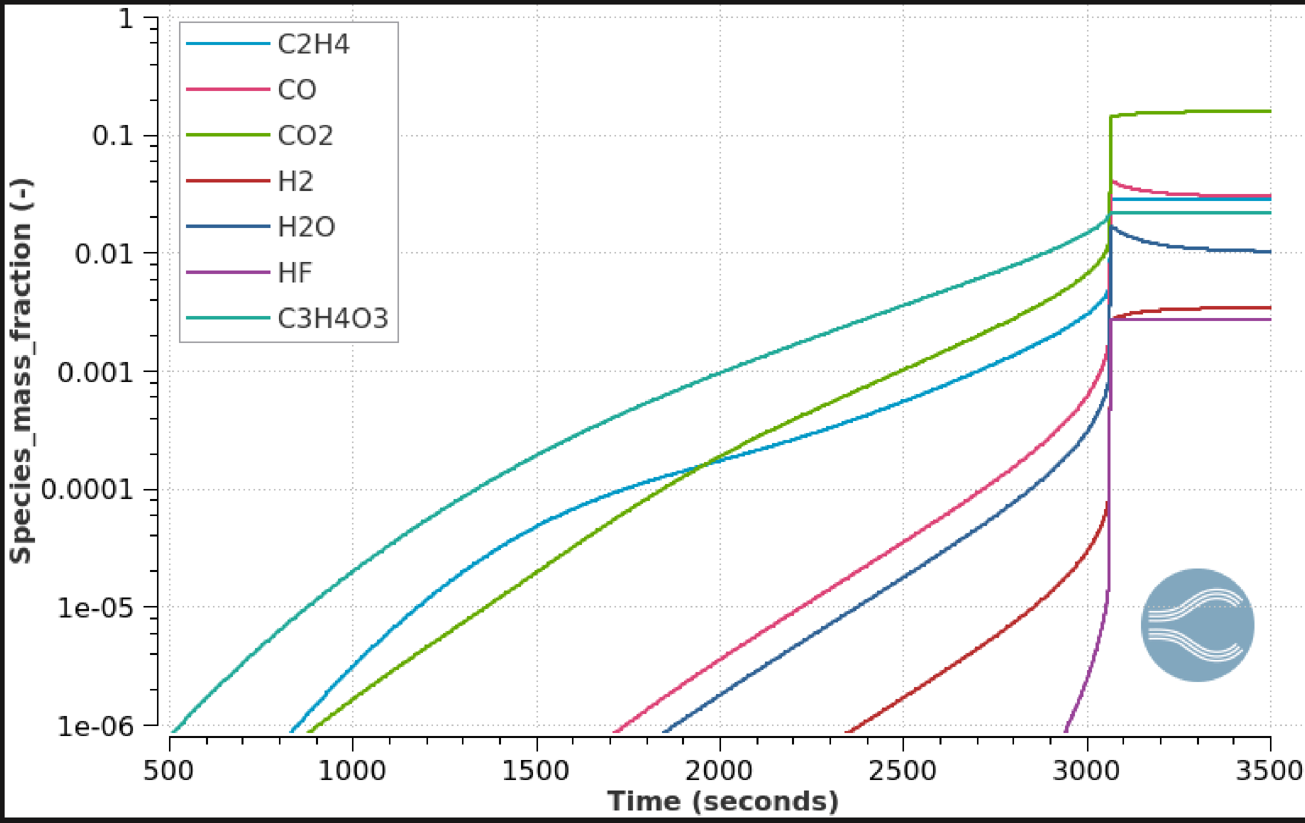
Niklas Weber, Sebastian Schuhmann, Jens Tübke, and Hermann Nirschl*

Description	Chemical equation	Reaction Enthalpy [kJ mol^{-1}]	Reference
Anode main reaction	$2LiC_6 + C_3H_4O_3 -> Li_2CO_3 + C_2H_4 + 2C_6$	−281.4	[7]
LiF formation	$Li_2CO_3 + PF_5 -> 2LiF + POF_3 + CO_2$	−77.1	[7,44,45]
Li_2O_2 formation	$Li_2CO_3 \rightarrow Li_2O + CO_2$	222.6	[7,46]
Cathode, full oxidation	$5MO_2 + C_3H_4O_3 -> 5MO + 3CO_2 + 2H_2O$	−201.5	[23,32]
Cathode, partial oxidation	$5MO_2 + 3C_3H_4O_3 -> 5MO + 6CO + 4H_2 + 3CO_2 + 2H_2O$	−105.5	[23,32]
Salt decomposition	$LiPF_6 -> LiF + PF_5$	84.27	[45]
Solvent decomposition	$n\,C_3H_4O_3 -> (CH_2CH_2O)_n + n\,CO_2$		
Solvent evaporation	$C_3H_4O_3(l) -> C_3H_4O_3(g)$	60.8	[7]
HF formation	$POF_3 + 3H_2O -> 3HF + H_3PO_4$	−123.4	[44,47]
Water–gas shift	$CO + H_2O \rightleftharpoons CO_2 + H_2$	−41.2	[44]

$$r_i = k_i \prod_j x_j^{a_{j,i}}$$

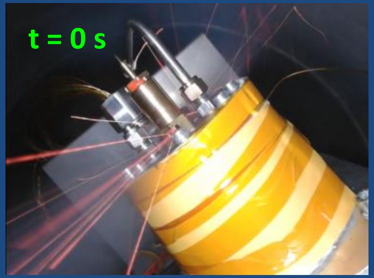
$$k_i = A_i \exp\left(-\frac{E_i}{RT}\right)$$

$$\frac{dx_j}{dt} = \sum_i \nu_{i,j} r_i$$



- A comprehensive species-based reaction mechanism for thermal runaway chemistry? : COMPUTATIONAL CHEMISTRY CONSORTIUM

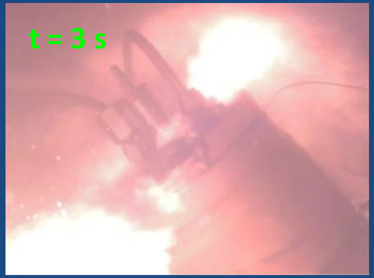
Ambient Gas Composition Impacting Propagation



First sparks resulting from nail penetration visible

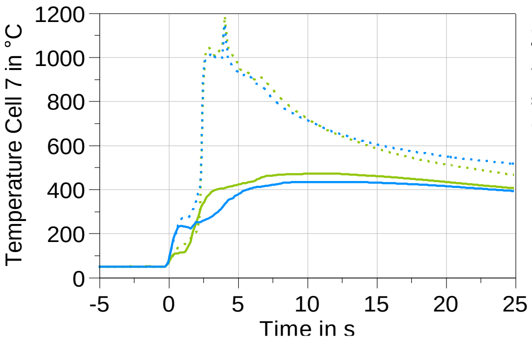
Thermal runaway with sparks and flames

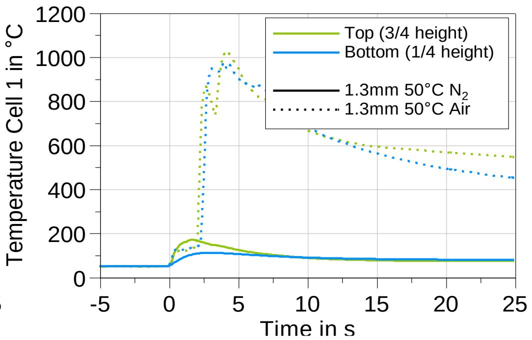
Ignition of large amounts of air/venting gas mixture

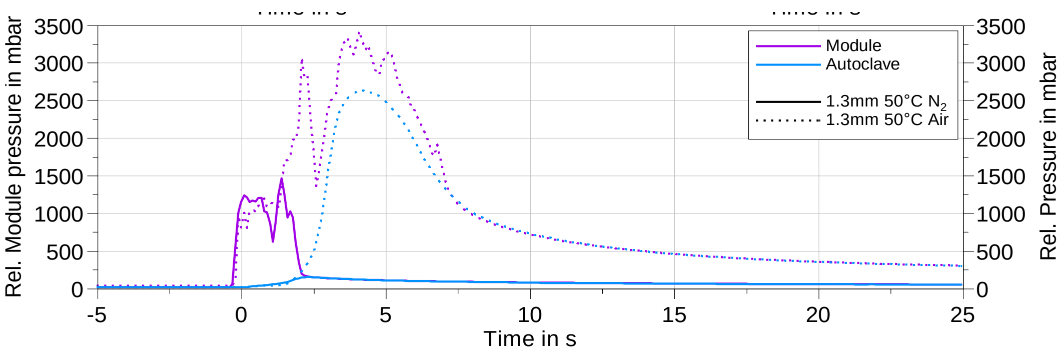


Diffusive combustion of air/venting gas mixture

Thermal runaway with sparks and flames

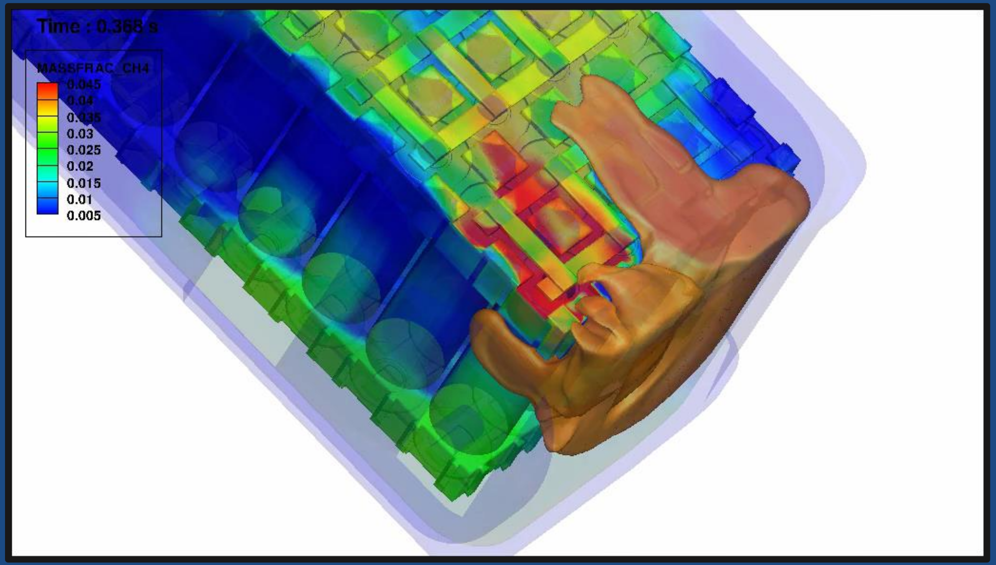




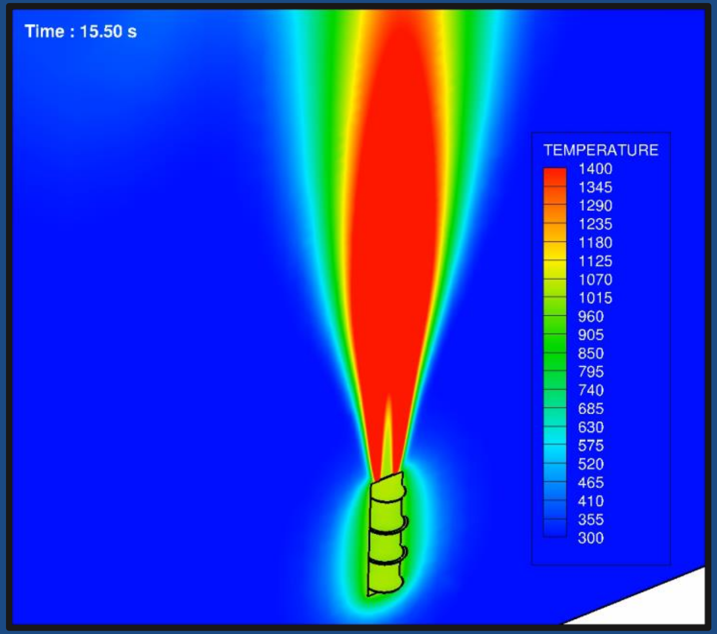


- Fundamentally different behaviour between N_2 and Air as ambient gas
- Vent gas combustion with air ambient gas leads to full propagation within 10s

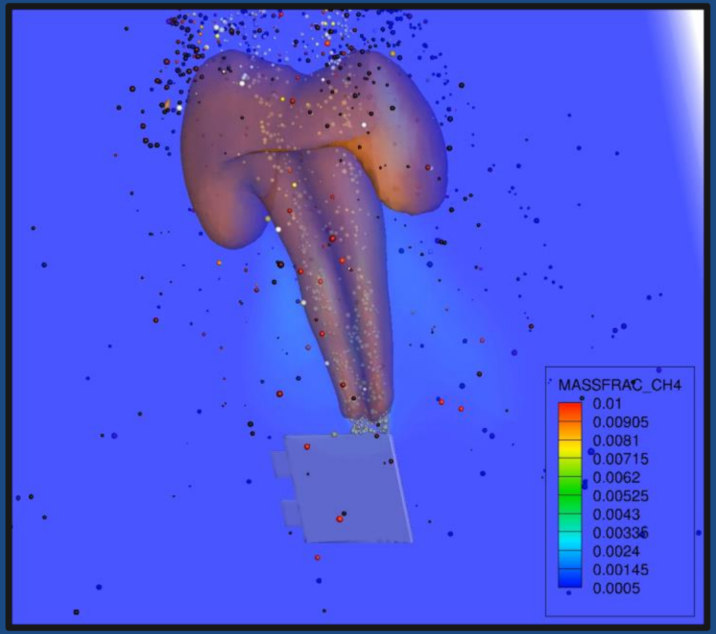
Battery Vent Gas Ignition and Combustion



Spark ignited vent gas combustion inside a battery pack



Self ignition of vent gases after exit

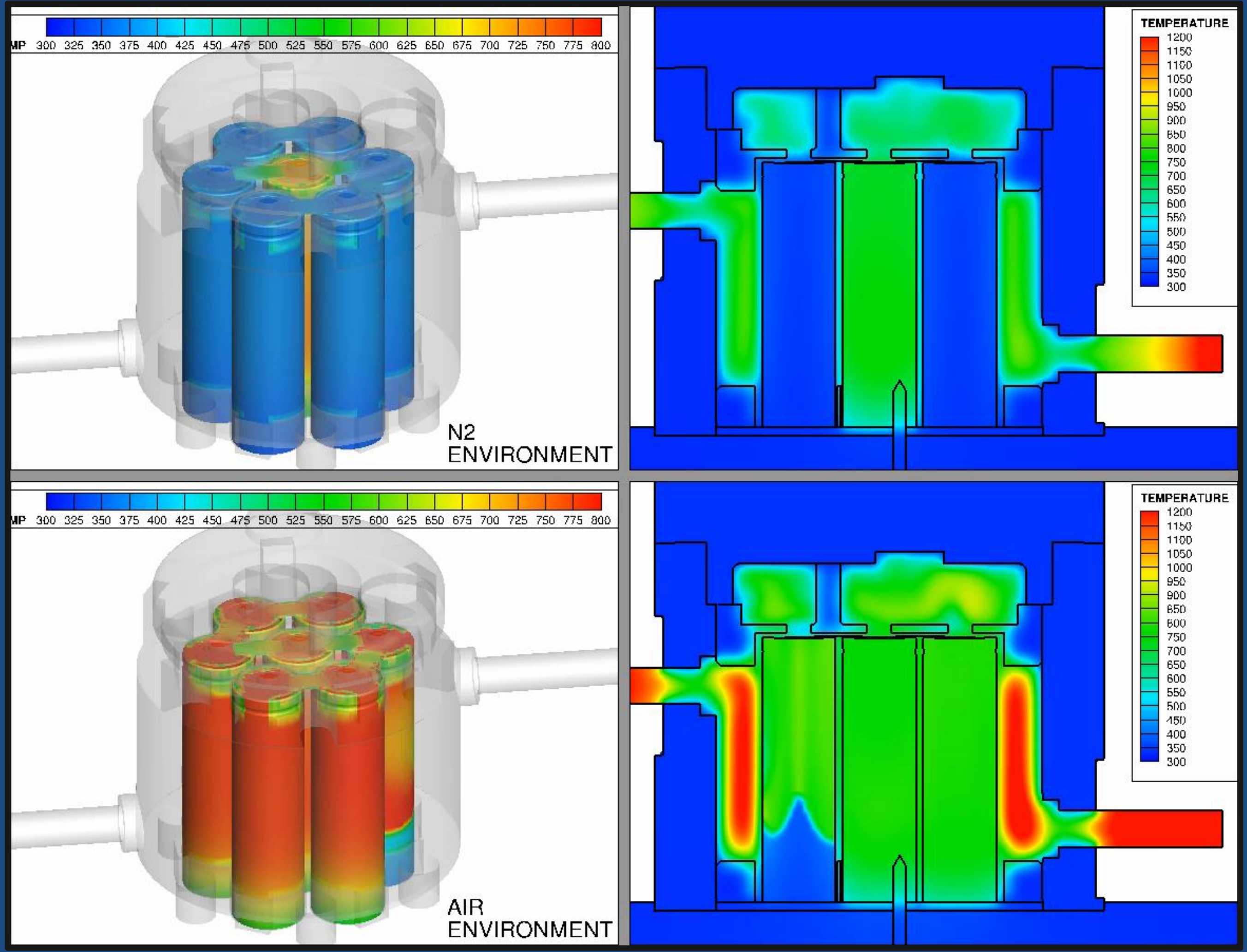


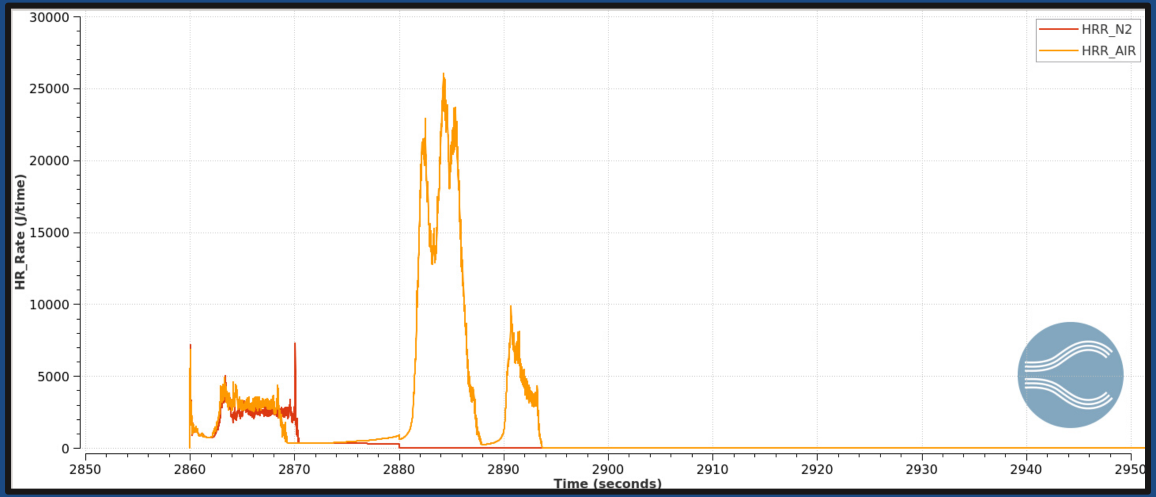
Vent gas ignition due to hot ejecta

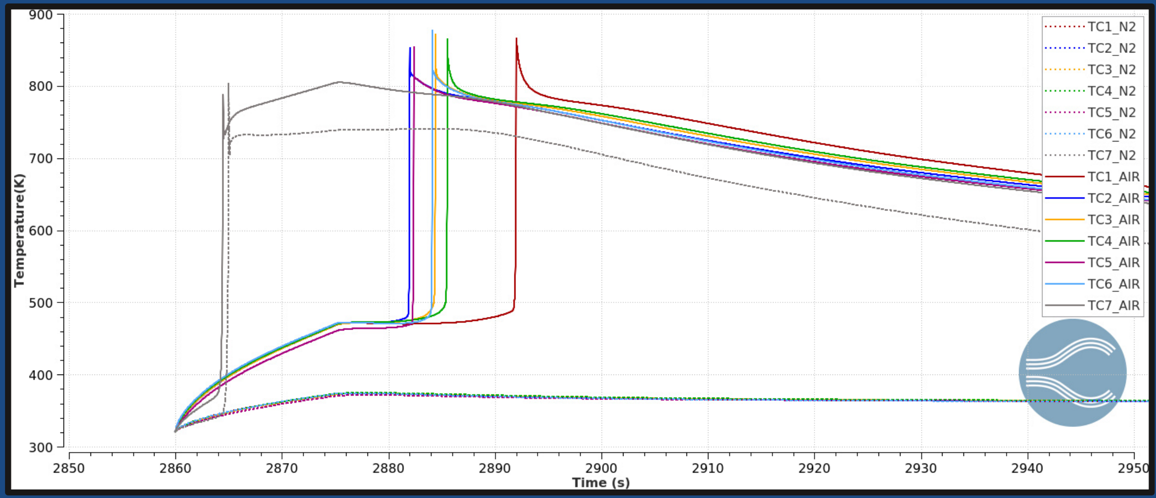
Gas-phase dynamics

With N2 environment : No TRP, No combustion event
With AIR environment : Quick TRP, Violent combustion event

Experimental behavior reproduced using CONVERGE simulations
Simplified approach to model vent gas combustion : Species sourcing
- N2 environment : Hot vent gas species at venting temperatures
- AIR environment : Hot combustion products at burned gas temperatures (evaluated using zero-D CONVERGE simulations)







THANK YOU!

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