Capturing Battery Thermal Runaway and Venting Phenomena using Detailed 3D CFD Solutions

Kislaya Srivastava[1], Tristan Burton[1], Daniel Probst[2]

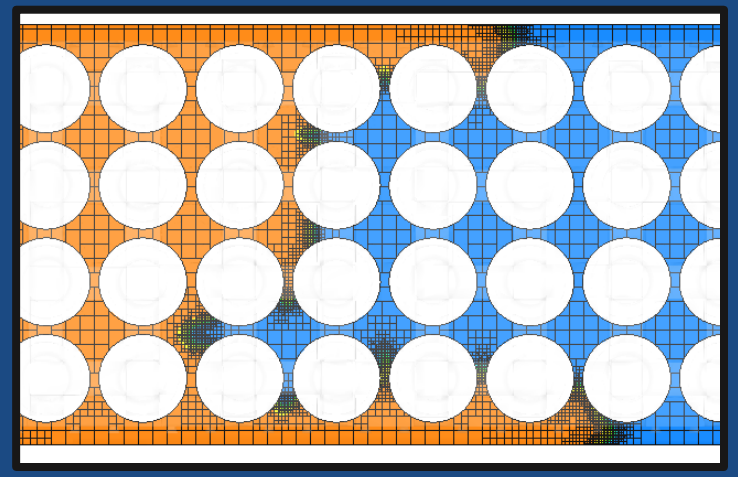
[1]Convergent Science Inc., Northville, MI 48167

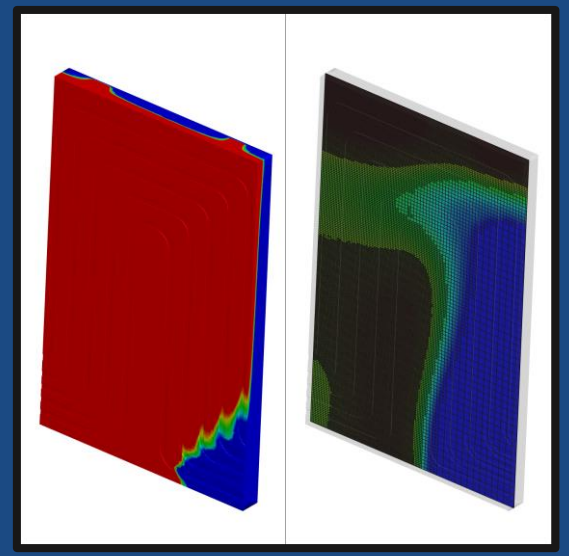
[2]Convergent Science Inc., Madison, WI 53719

CONVERGENT SCIENCE

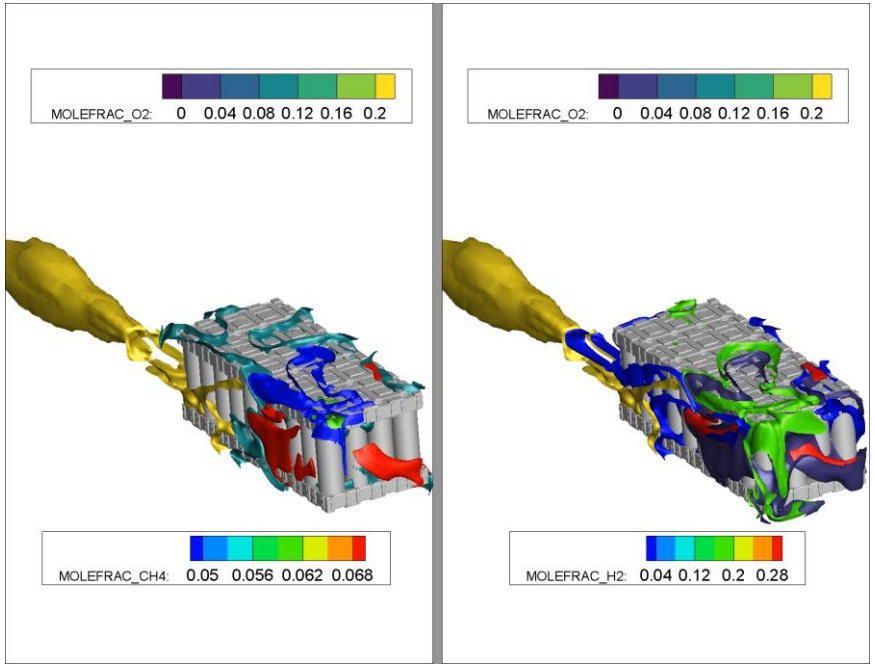
Combustion using Detailed chemistry and AMR

- CONVERGE contains the SAGE detailed chemical kinetics solver, parallelized efficiently for fast run-times
- The SAGE detailed chemistry solver is efficient, even with a large mechanism
- Uses local conditions to calculate reaction rates based on principles of chemical kinetics
- Autonomous meshing is well-suited for complex geometries, eliminating user meshing time
- Adaptive mesh refinement (AMR) automatically resolves the flow, diffusion of vent gas, flame front and thermal runaway front propagation at low computational expense

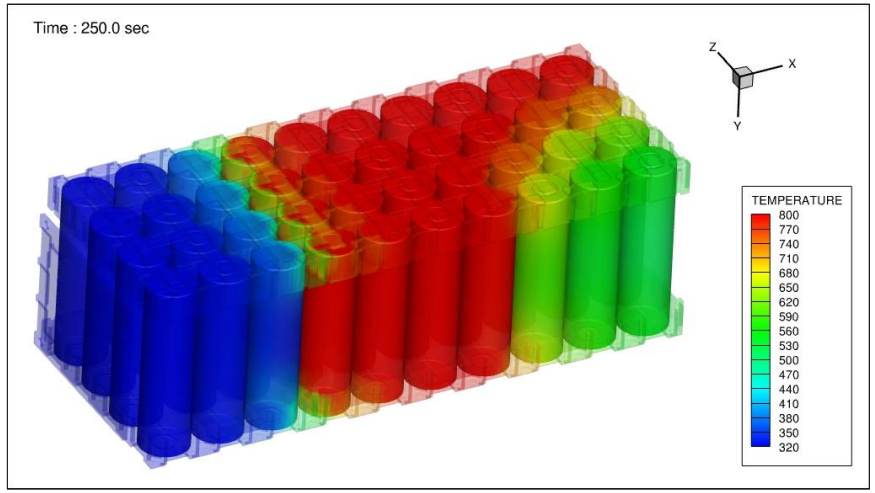




Thermal Runaway Propagation and Vent Gas Analysis



CFD Modeling of Battery Thermal Runaway and Vent Gas Ignition Using Detailed Chemistry,
Tristan Burton,
2020 NASA Aerospace Battery Workshop



CFD Modeling of Battery Thermal Runaway Propagation using Detailed Chemistry,
Kislaya Srivastava et.al,
2021 NASA Aerospace Battery Workshop

Sample Thermal Runaway Mechanisms in CONVERGE

HATCHARD-KIM TR MECHANISM

- 4 Reactions, LCO battery chemistry
  - Kim et al., 2007

SEI decomposition (sei)

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

Anode and electrolyte (ne)

$$R_{ne}(T, c_e, c_{neg}, t_{sei}) = A_{ne} \exp\left[-\frac{t_{sei}}{t_{sei,ref}}\right] c_{neg}^{m_{ne,n}} \exp\left[-\frac{E_{a,ne}}{RT}\right]$$

Cathode and electrolyte (pe)

$$R_{pe}(T, \alpha, c_e) = A_{pe} \alpha^{m_{pe,p1}} (1-\alpha)^{m_{pe,p2}} \exp\left[-\frac{E_{a,pe}}{RT}\right]$$

Electrolyte decomposition (e)

$$R_e(T, c_e) = A_e \exp\left[-\frac{E_{a,e}}{RT}\right] c_e^{m_e}$$

REN TR MECHANISM

- 6 Reactions, NMC battery chemistry
  - Ren et al., 2018

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

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

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

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

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

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

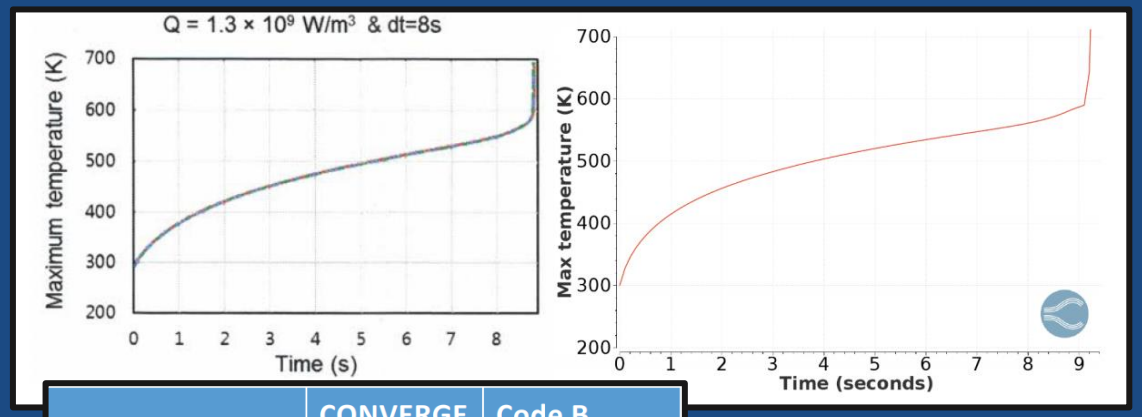
$$c_{Cat} = 1 - \int \kappa_{Cat} dt$$

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

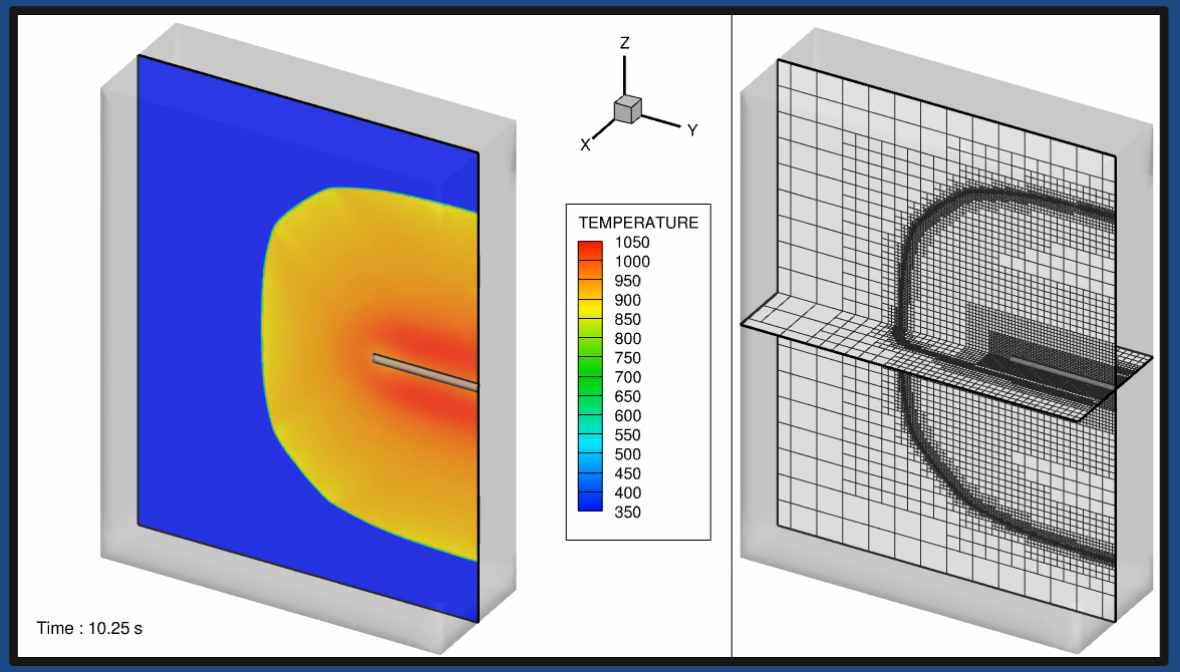
SEI film decomposition (SEI)
Anode and electrolyte (An-E)
Anode and binder (An-B)
Cathode and anode (Cat-An)
Cathode and binder (Cat-B)
Cathode decomposition (Cat)

Thermal Runaway using Detailed chemistry and AMR

- Thermal runaway initiated through nail penetration into a prismatic LCO-type battery
  - Initial heat release due to short-circuiting specified
  - KIM TR mechanism employed for heat release within solid
  - Temperature-based adaptive mesh refinement (AMR) to closely track propagation
- Comparison to Zhang et al. (2020)

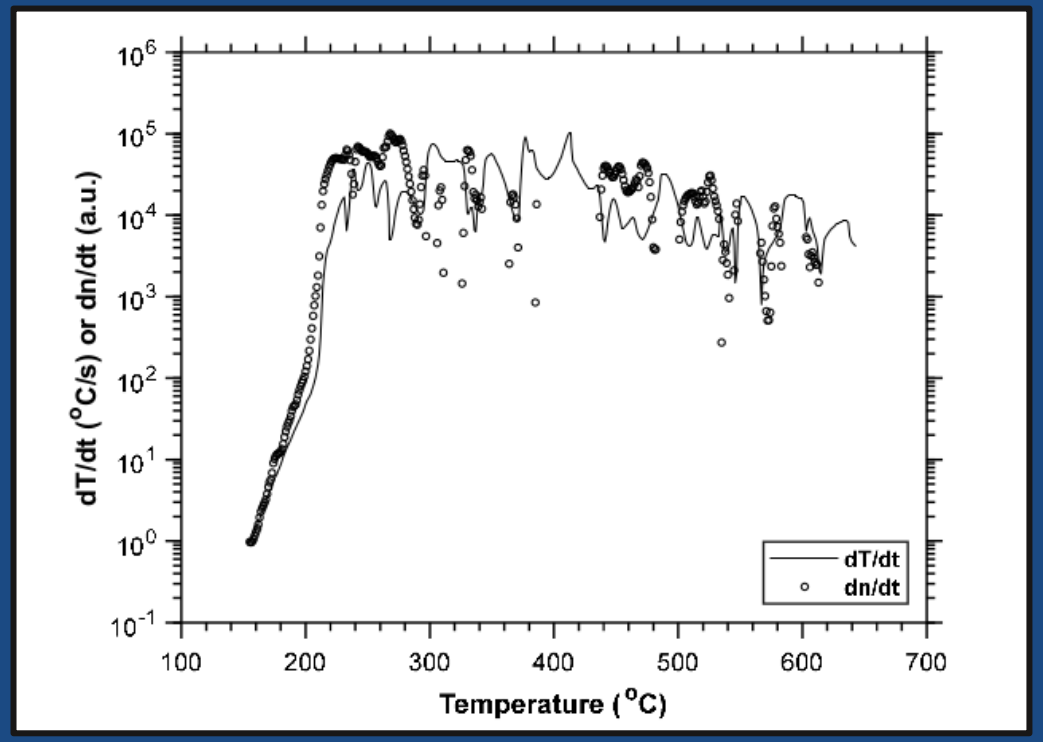


	CONVERGE	Code B
Cell Count	91972	68240
Cell Sizes (mm)	0.7:10	0.7:10
Runtime (4 cores)	0.47 hours	6 hours

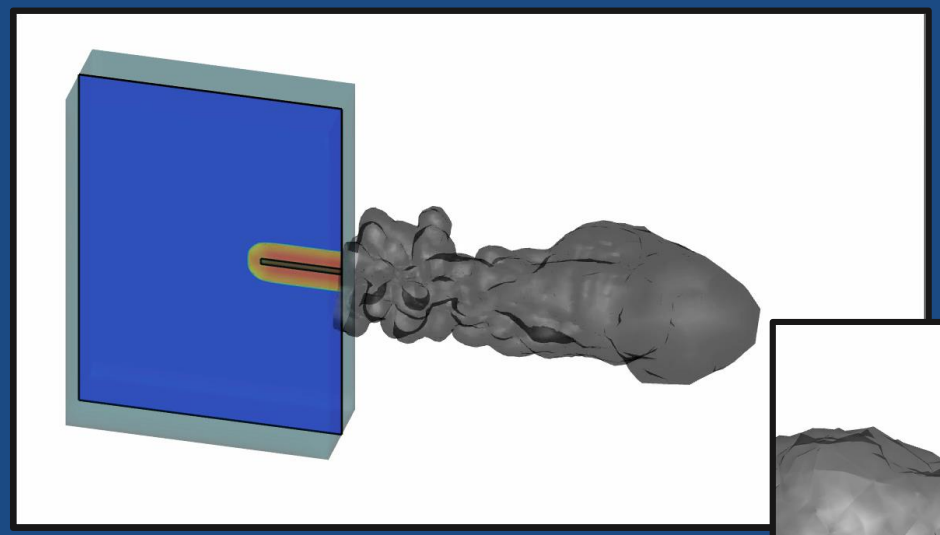


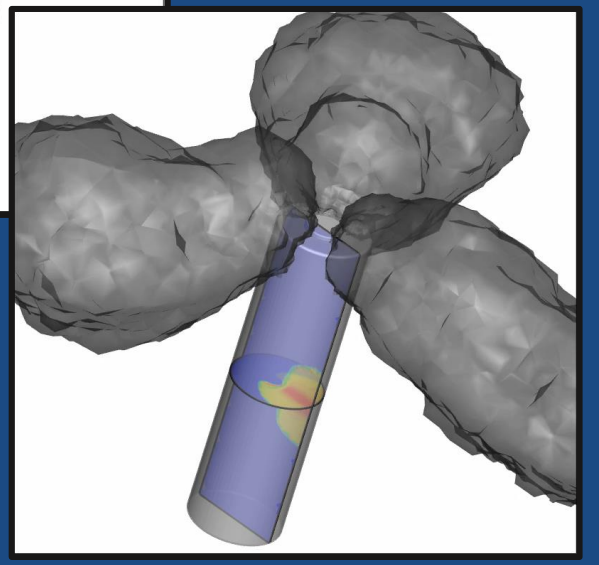
Coupling Thermal Runaway and Vent Gas Generation

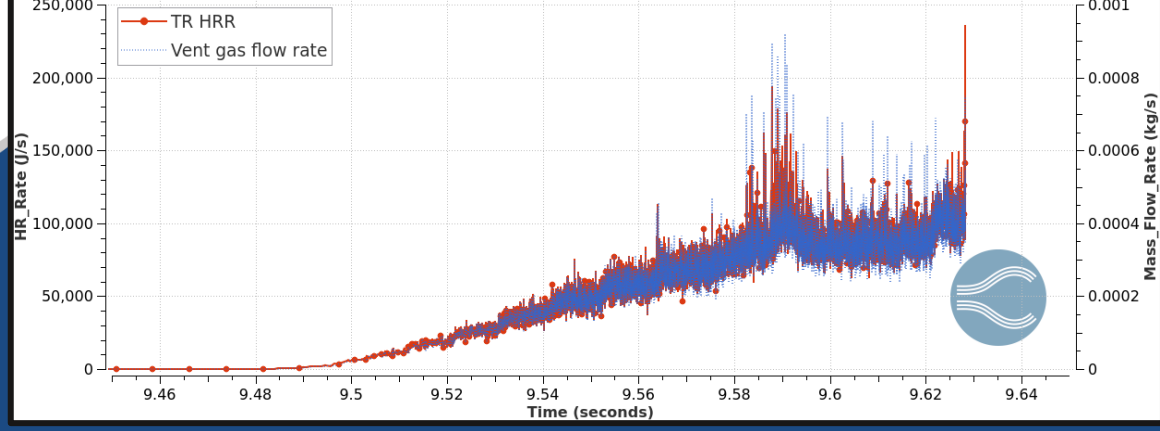
- Vent gas generation proportional to TR reaction rates



Cell heating rate and gas generation rate based on calorimetry measurements for an 18650 LCO cell (Ostanek et al., Jhu et al.)







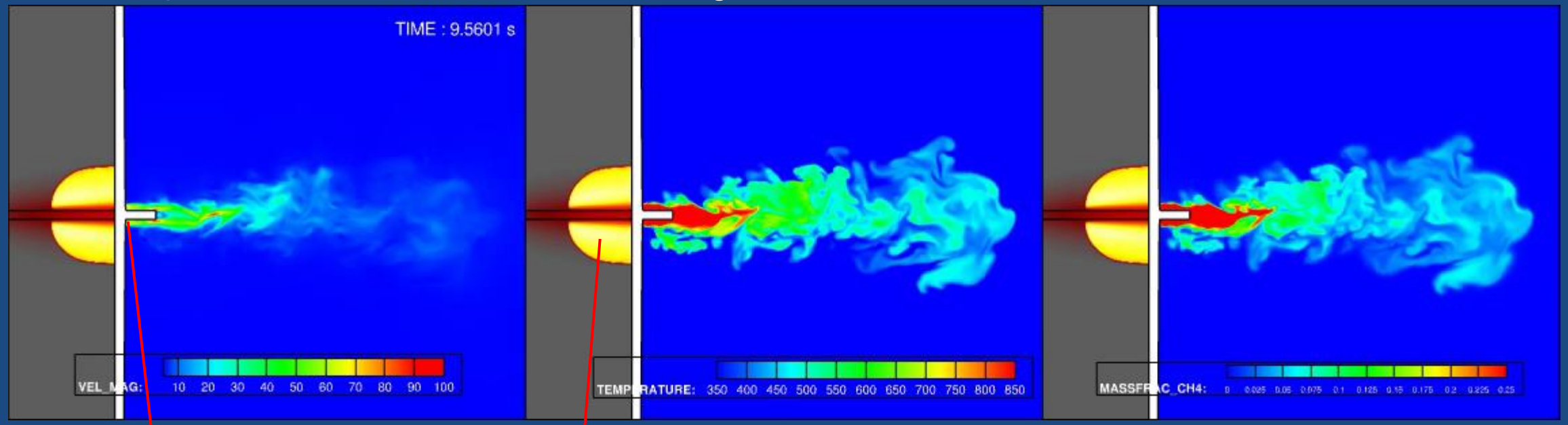
Option1: Solid-Gas Coupled TR

- TR predictions in solid streams coupled with vent INFLOW conditions in fluid streams

Vent gas flow rate
$\dot{m}_{vg} = f(HRR_{TR}, R_j)$

Vent gas temperature
$T_{vg} = f(T_{Bat})$

Vent species composition
$Y_i = f(\dot{c}_{SEI}, \dot{c}_{AN}, \dot{c}_{CAT}, \dot{c}_{ELE}, \ldots)$

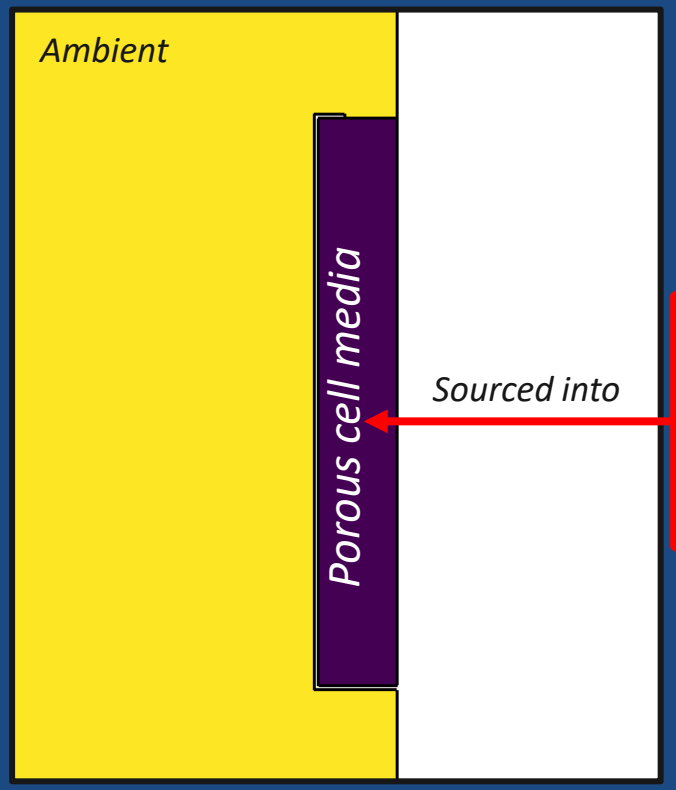


Gas INFLOW BC ← coupled with → TR mechanism predictions in Solid

Option2: Porous Media Approach (1/2)

- Modelling the battery solid as a gaseous porous volume
  - Based on model presented by Kim et. al., "*Modeling cell venting and gas-phase reactions in 18650 lithium ion batteries during thermal runaway*"
  - Model gas pressure within the battery porous volume
  - Change in porous solid density also incorporated

$$\frac{d\alpha}{dt} = -A_{ab}(\alpha)^m(1-\alpha)^n \exp\left(-\frac{E_{a,ab}}{RT}\right)\exp(-B_{ab}\alpha)$$



One-step lumped thermal abuse reaction

$$cell \rightarrow x\ volatiles + (1-x)\ remains$$

- Assumptions: All volatile gases quickly relaxes to equilibrium compositions measured in the experiments

Mass Source: $\dot{S}_{m,ab} = xW\frac{d\alpha}{dt}$

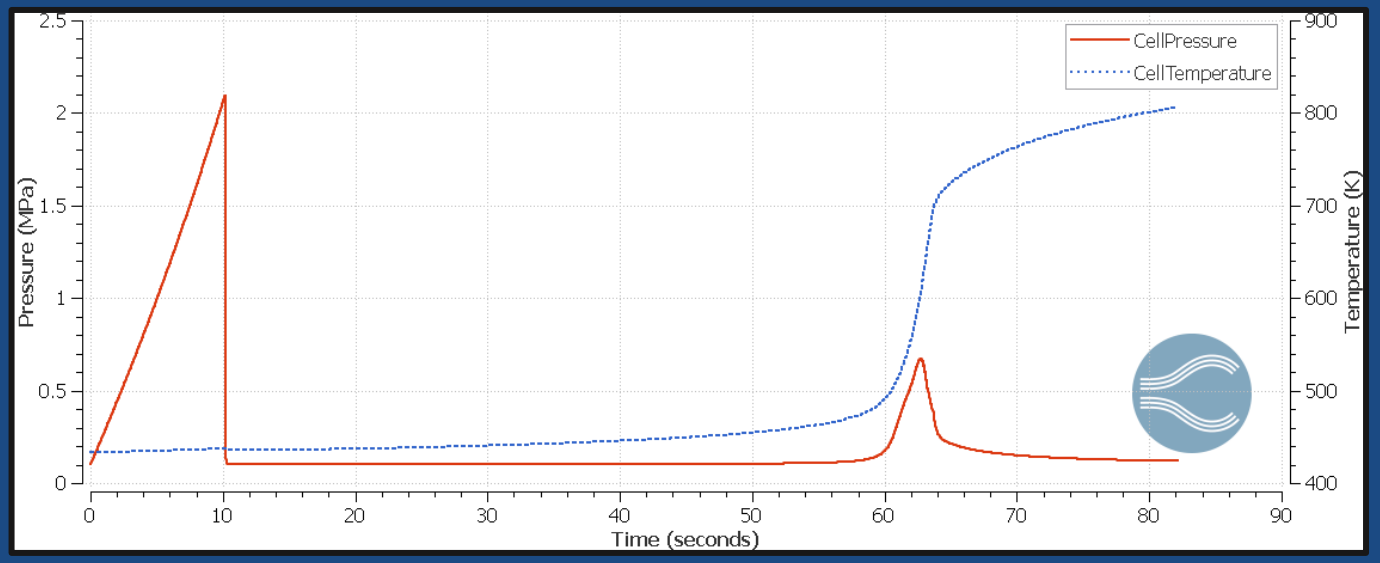
Species Source: $\dot{S}_{g,i,ab} = Y_{i,eq}\dot{S}_{m,ab}$

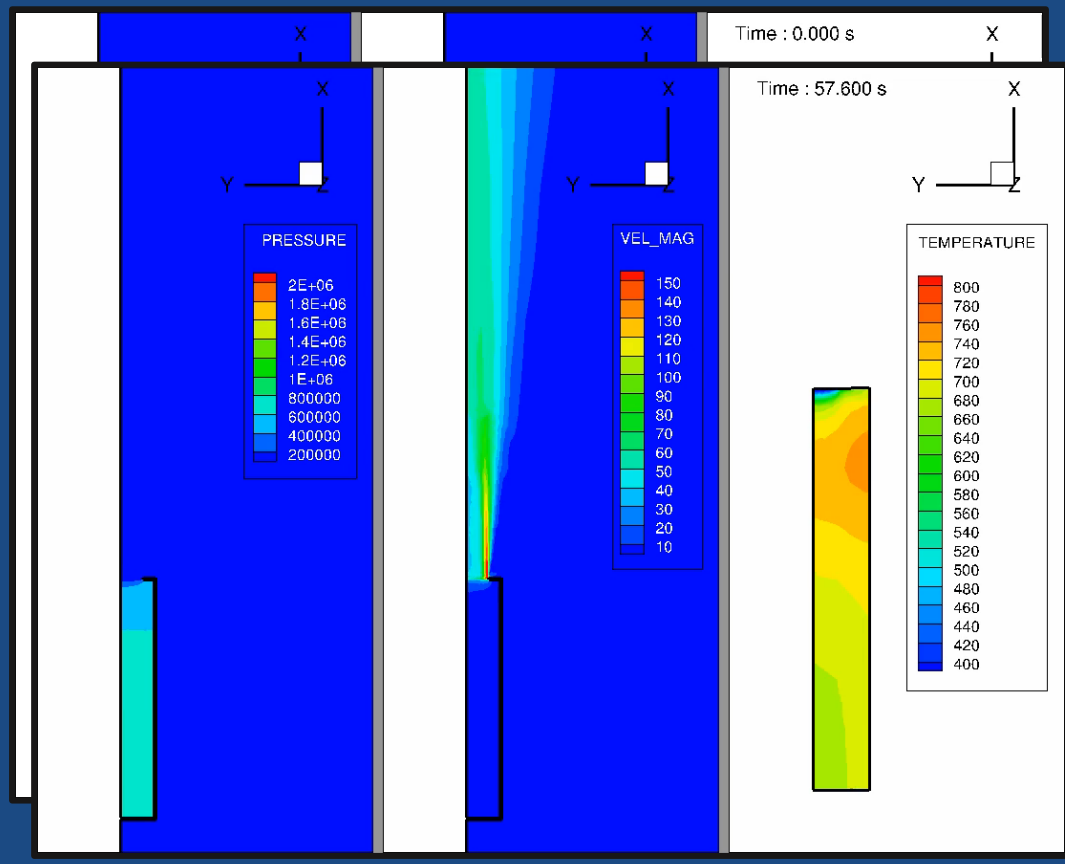
Heat Source: $\dot{S}_{heat,ab} = H_{ab}\frac{d\alpha}{dt}$

(α = degree of conversion)

Option2: Porous Media Approach (2/2)

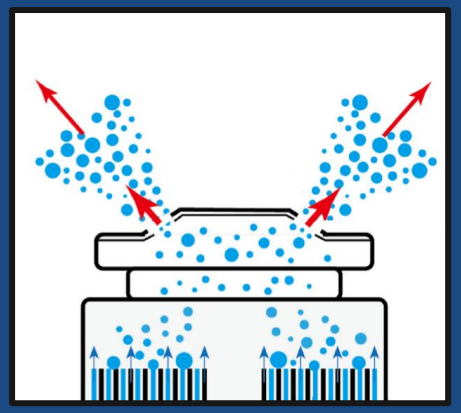
- First venting stage :
  - Pressure controlled event for cell cap burst
- Second venting stage :
  - Rapid gas generation due to thermal runaway





Option3: Lumped Battery Pressure Modeling (1/2)

- Based on model presented by Ostanek et. al., "*Simulating Onset and Evolution of Thermal Runaway in Li-ion Cells using a Coupled Thermal and Venting Model*"
  - Vent gas mass generation coupled to individual TR reaction rates. Electrolyte vaporization can be included
  - Lumped pressure evaluated inside the battery
  - Use Option1 type setup to feed mass flow rates calculated as a function of pressure ratio across vent



V_h : *Headspace Volume*
T_{cell}: *Mean temperature of battery*
R_j : *TR rxn rate of* j^{th} *rxn*
Δm_j : *Mass of vent gas from* j^{th} *rxn*

Calculating pressure inside the battery :

Equation of state :

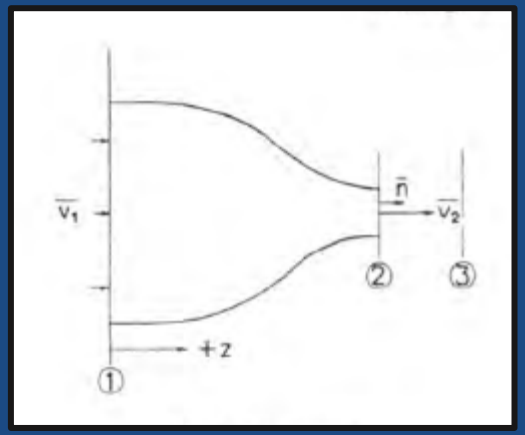
$$P_{ventgas} = \frac{m_{ventgas} R_{ventgas} T_{cell}}{V_h}$$

$$\frac{dm_{ventgas}}{dt} = \dot{m}_{vent} + \sum \dot{m}_{gen}$$

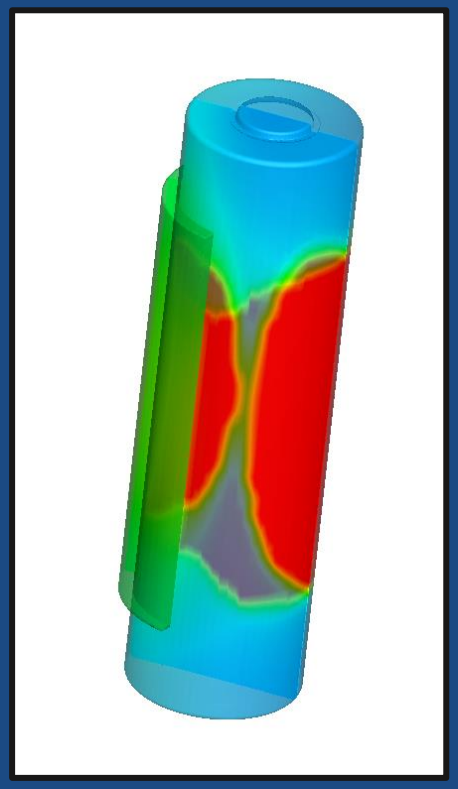
$$\dot{m}_{gen,j} = \Delta m_j R_j$$

Calculating mass flow rate, temperature out of vent:

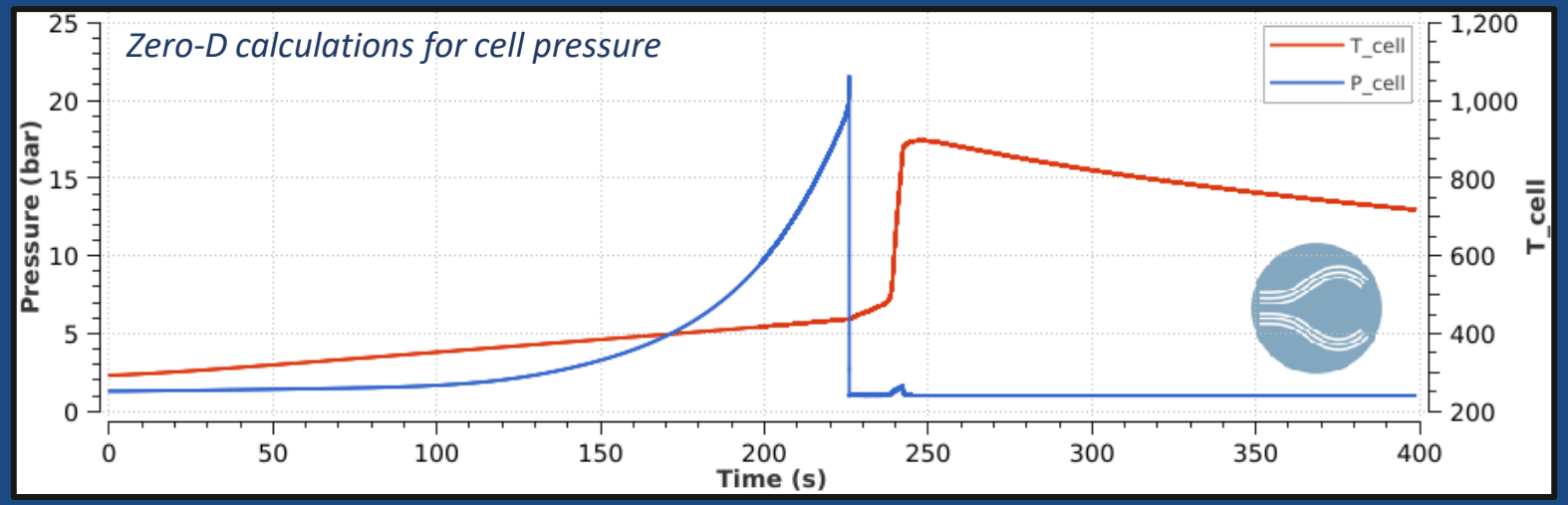
Isentropic, adiabatic equations for flow through a sharp edge orifice : $\dot{m}_{vent}$

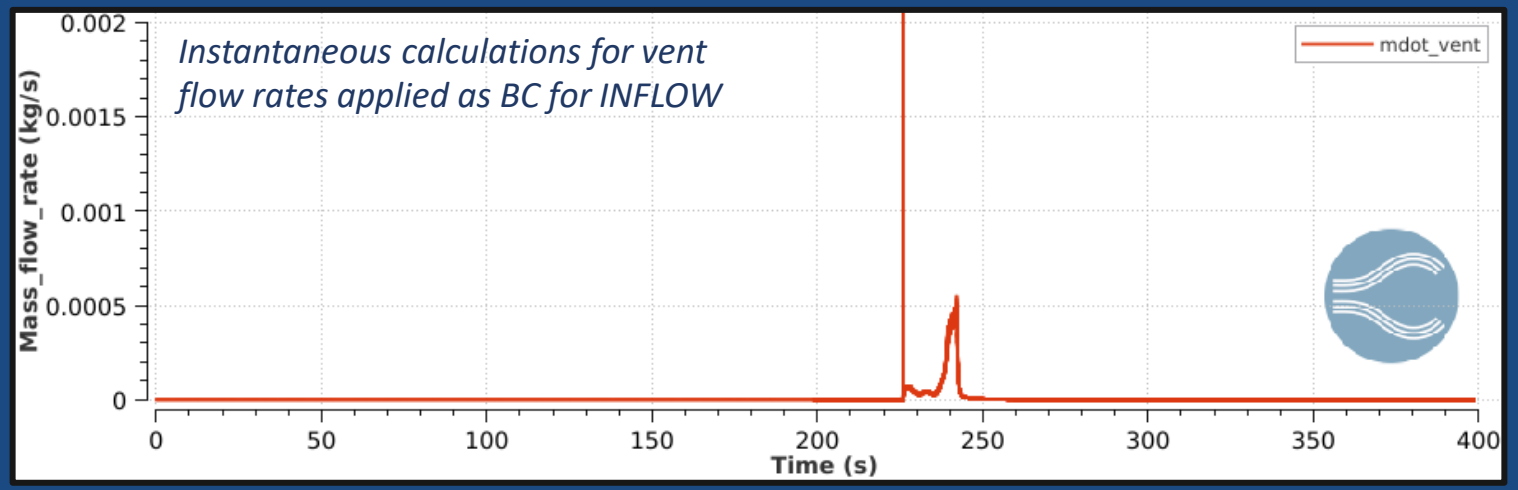


Option3: Lumped Battery Pressure Modeling (2/2)

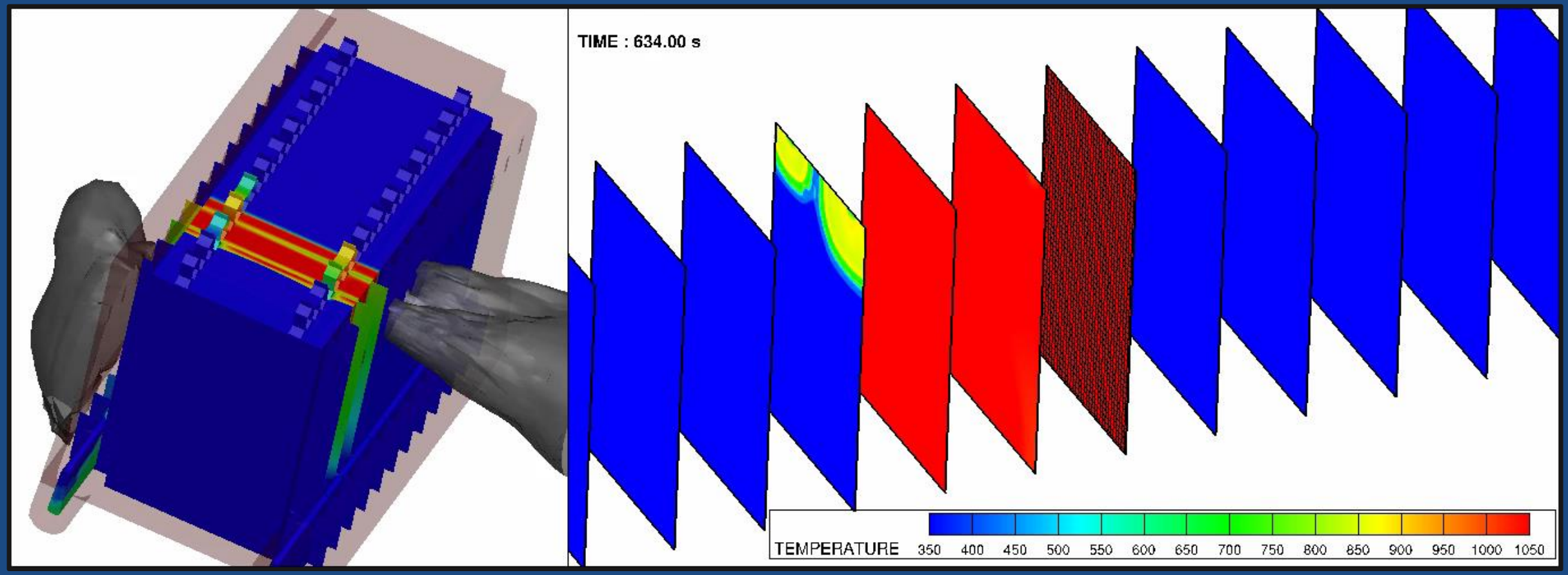


Results shown are from a solid-only TR simulation

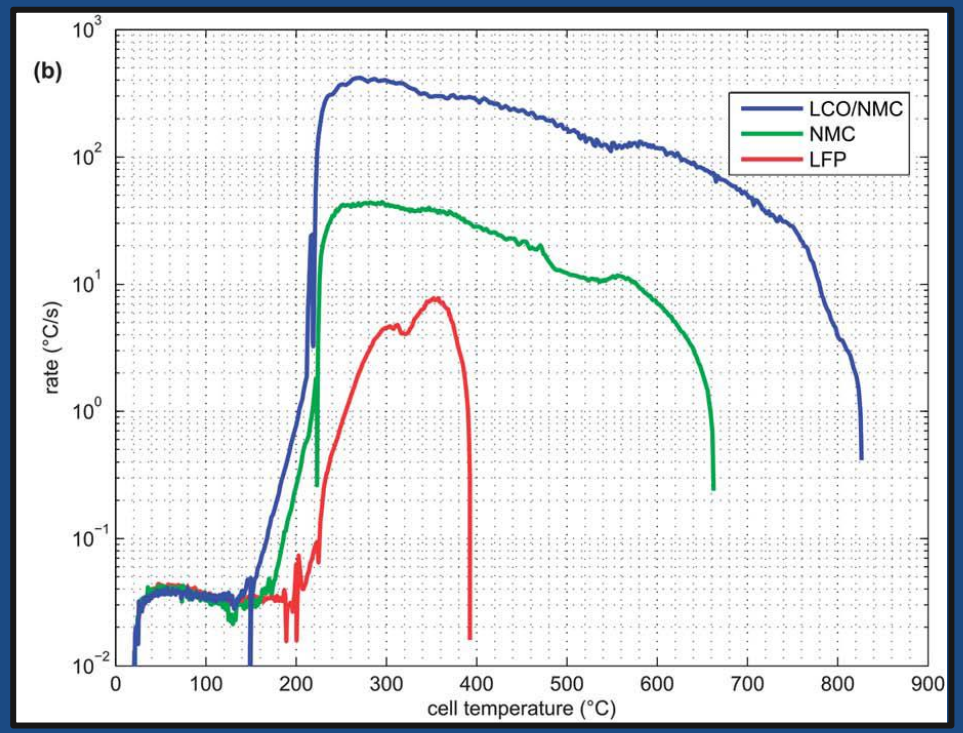




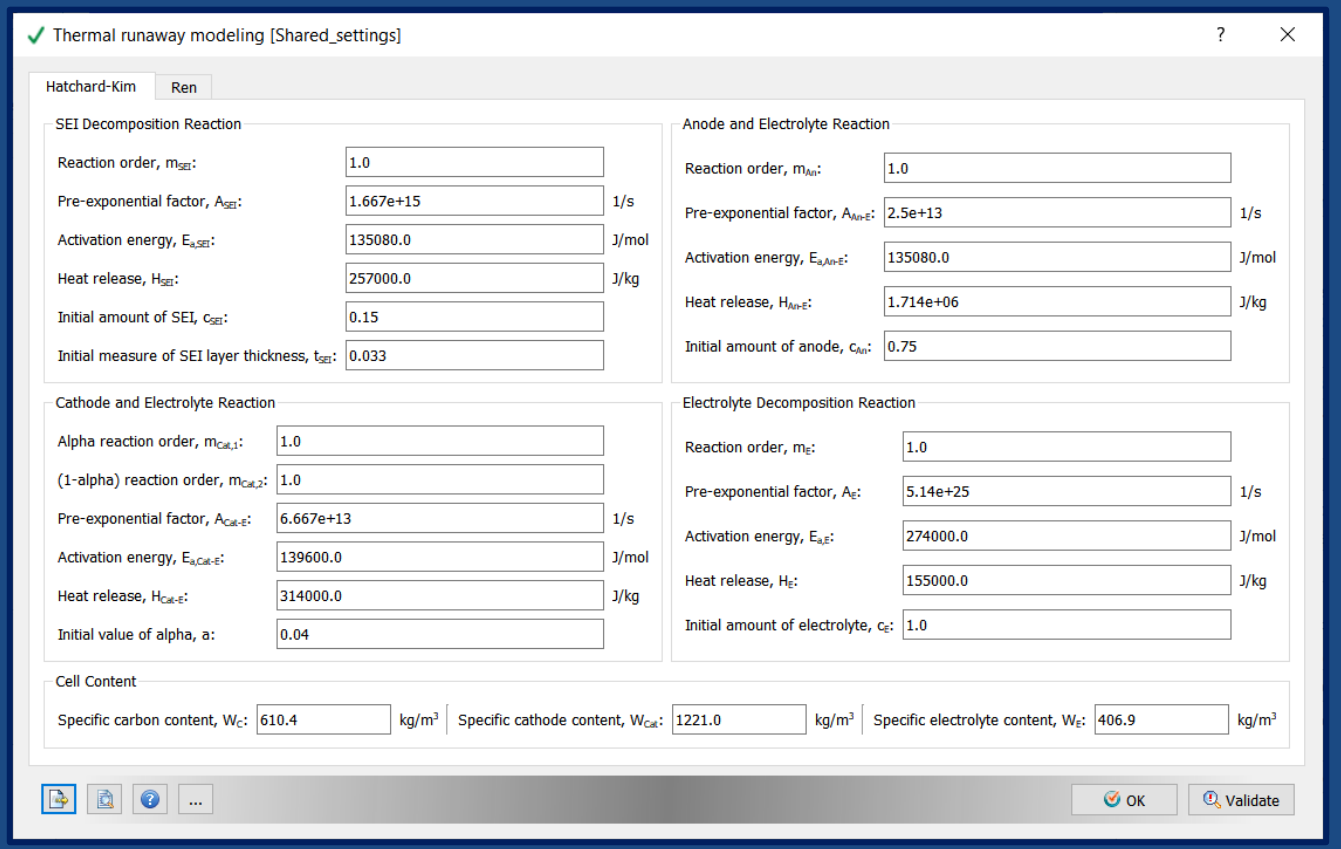
Coupled Thermal Runaway and Venting within a Pack



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*"

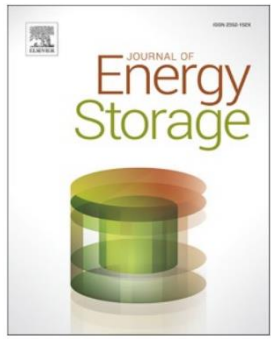


Experimental Studies on TR Behaviour

Cell-to-cell variability in Li-ion battery thermal runaway: Experimental testing, statistical analysis, and kinetic modeling

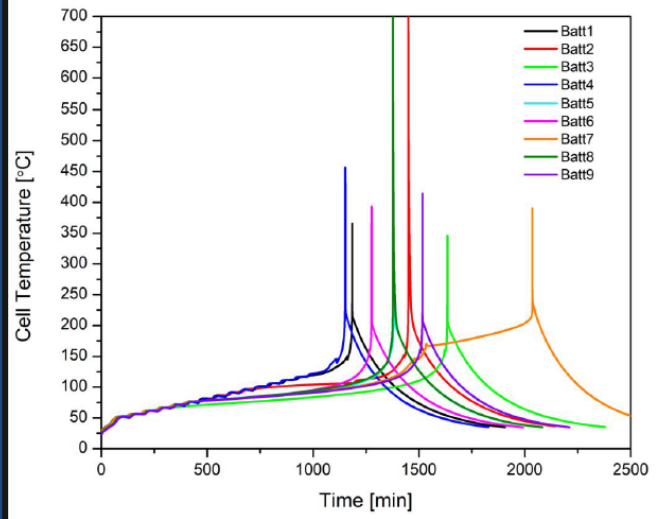
Liwen Zhang [a], Shiyou Yang [b], Lu Liu [a], Peng Zhao [a,*]

[a] Department of Mechanical, Aerospace & Biomedical Engineering, UT Space Institute, University of Tennessee, Knoxville, TN 37388, USA
[b] Ford Research and Advanced Engineering, Ford Motor Company, Dearborn 48121, MI, USA



Experimental identification of cell-to-cell variation in thermal runaway of Samsung 18650 LCO batteries

Raw data from the ARC experiment



	Exotherm onset Temp[1] T_{exo}(°C)	Thermal runaway onset Temp[2] T_{TR}(°C)	Max Temp[3] T_{max}(°C)	TR delay time (min)	Mass change (g)
Batt 1	118.17	211.36	365.38	204.33	N/A
Batt 2	97.73	210.06	716.45	720.5	26.967
Batt 3	67.38	199.98	345.13	1308.96	9.951
Batt 4	123.83	220.94	456.48	121.52	27.131
Batt 5	77.69	201.14	384.15	897.43	21.674
Batt 6	77.44	195.36	392.72	802.80	24.405
Batt 7	76.89	228.62	390.33	1584.35	7.054
Batt 8	77.54	200.65	726.68	911.74	23.718
Batt 9	77.47	204.19	414.42	1044.03	9.797

Statistical Studies of TR behaviour

Statistical analysis of frequency factor and global activation energy of all 18650 Samsung LCO cells.

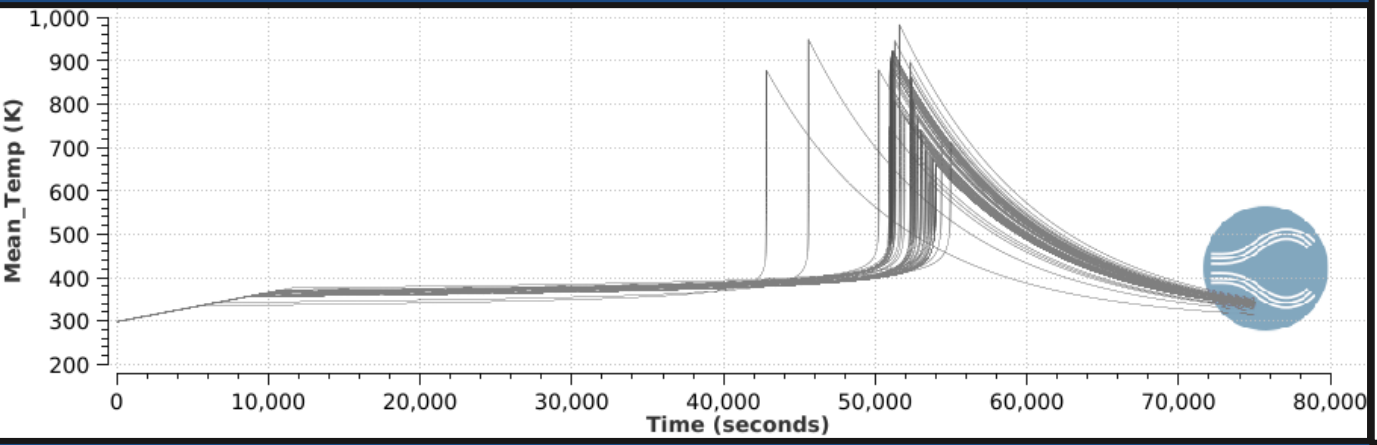
	ΔT_{ad} (K)	c_p (J/kg·K)	H (J/kg)	E (J/mol)	A (min^{-1})
Batt 1	247.2	730	1.80E5	9.65E4	2.00E9
Batt 2	618.7	730	4.52E5	9.33E4	4.10E8
Batt 3	277.8	730	2.03E5	8.30E4	9.00E8
Batt 4	332.6	730	2.43E5	8.39E4	4.50E7
Batt 5	306.5	730	2.24E5	8.03E4	3.77E7
Batt 6	315.3	730	2.30E5	8.33E4	1.06E8
Batt 8	649.1	730	4.74E5	8.24E4	2.99E7
Batt 9	336.9	730	2.46E5	8.36E4	7.40E7
Average	ΔT_{ave}: 385.5	c_{pave}: 730	H_{ave}: 2.29E5	E_{ave}: 8.58E4	A_{ave}: 3.49E8
Standard deviation	ΔT_{SD}: 156.3	c_{pSD}: 0	H_{SD}: 1.73E4	E_{SD}: 5.80E3	A_{SD}: 6.95E8

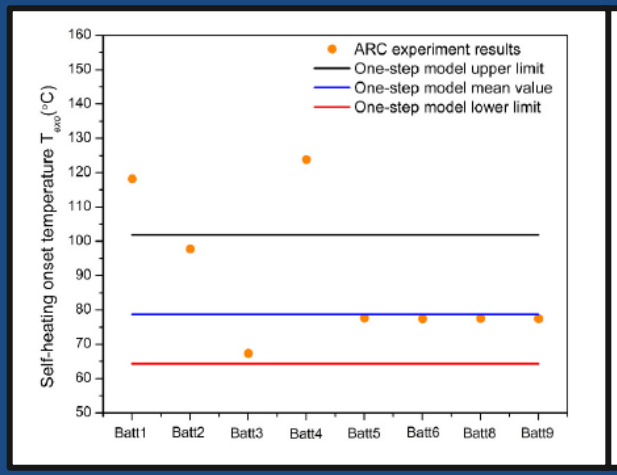
$$\frac{dc}{dt} = -Ace^{-\frac{E}{RT}}$$

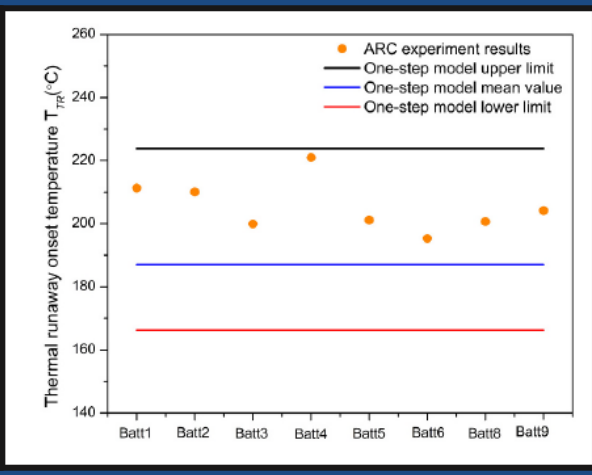
$$c_p\frac{dT}{dt} = HAce^{-\frac{E}{RT}}$$

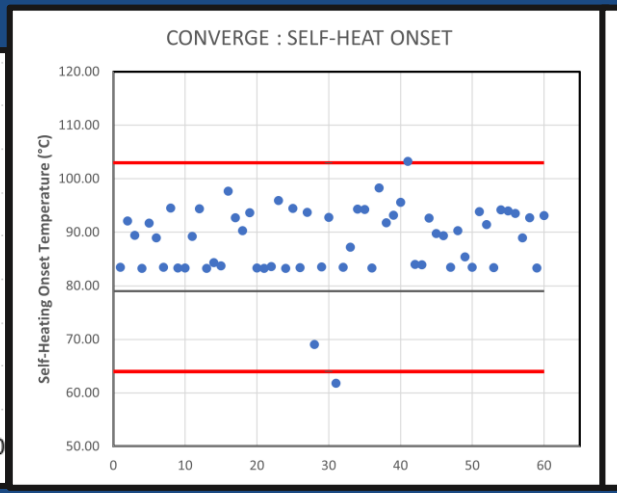
Zhang et. al. (2022)

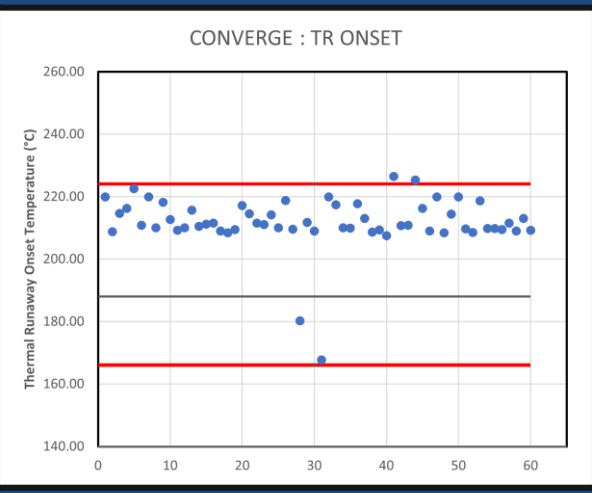
Randomized Activation Energy (E) value obtained from gaussian distribution of E_{ave} and E_{SD}
Pre-exponential factor (A) and Reaction enthalpy (H) interpolated from experimental data
A total of 60 design points simulated under ARC conditions



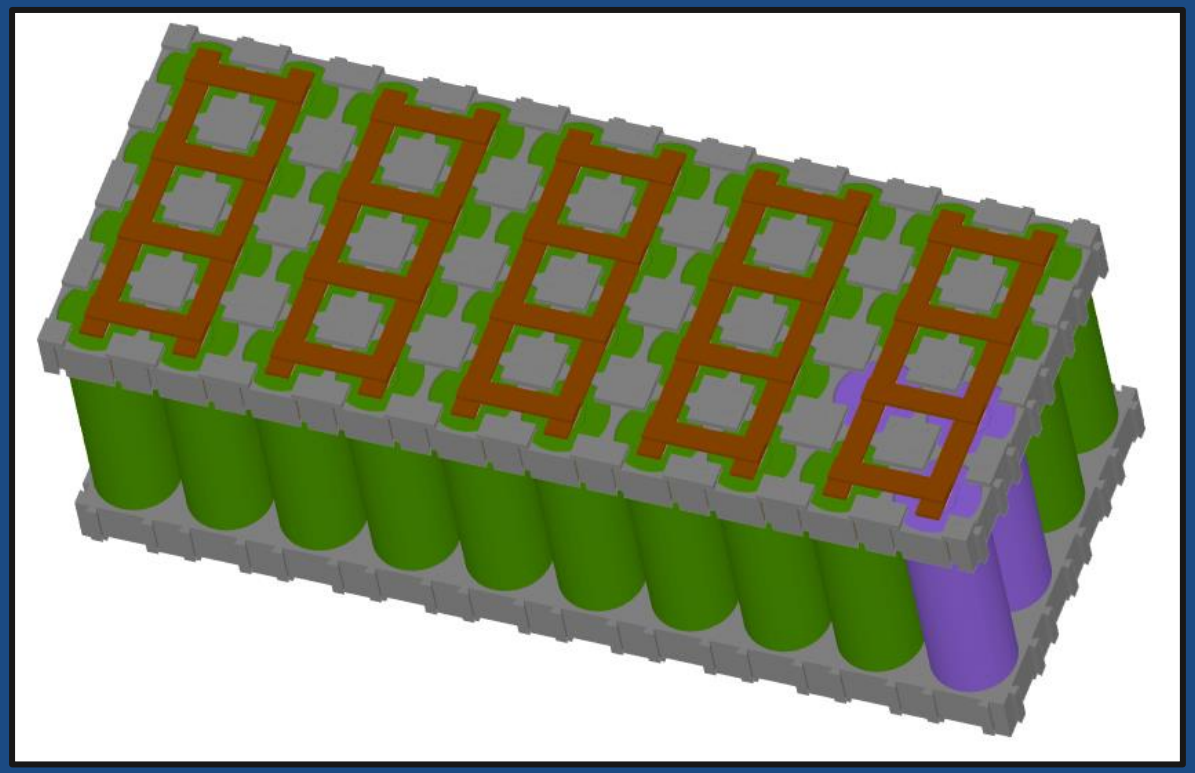


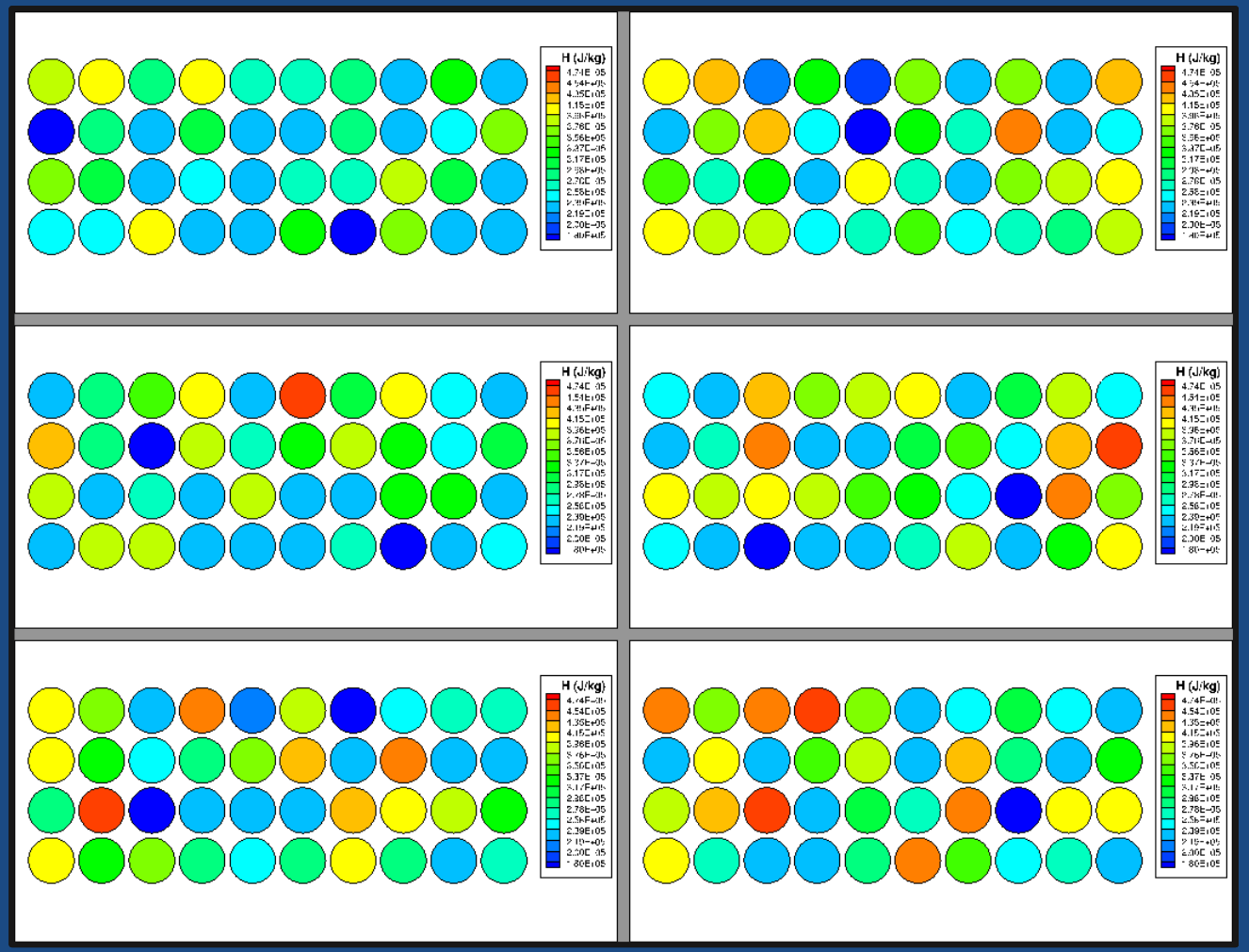






Statistical Studies of TR behaviour within pack (1/4)

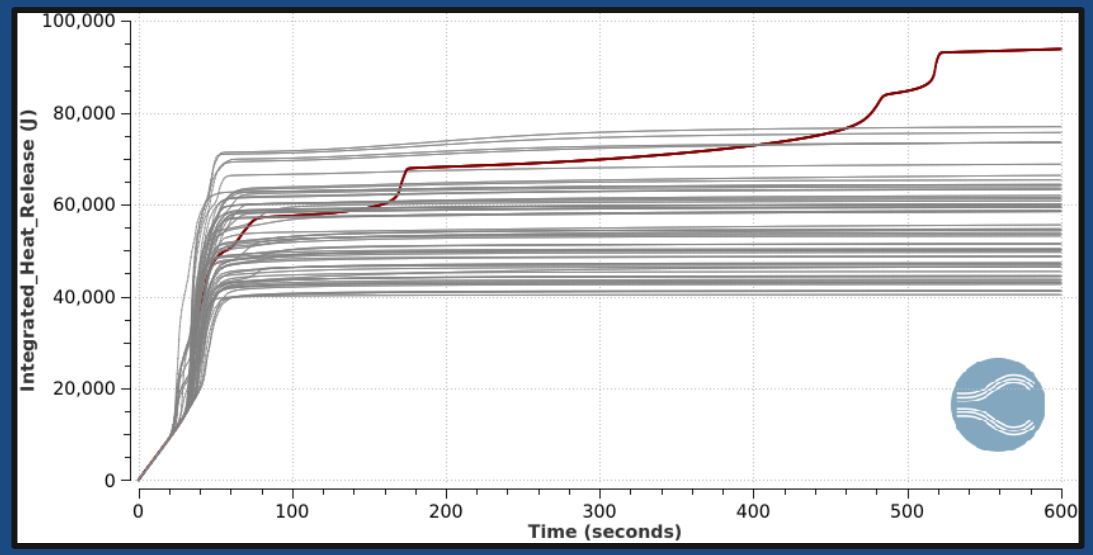




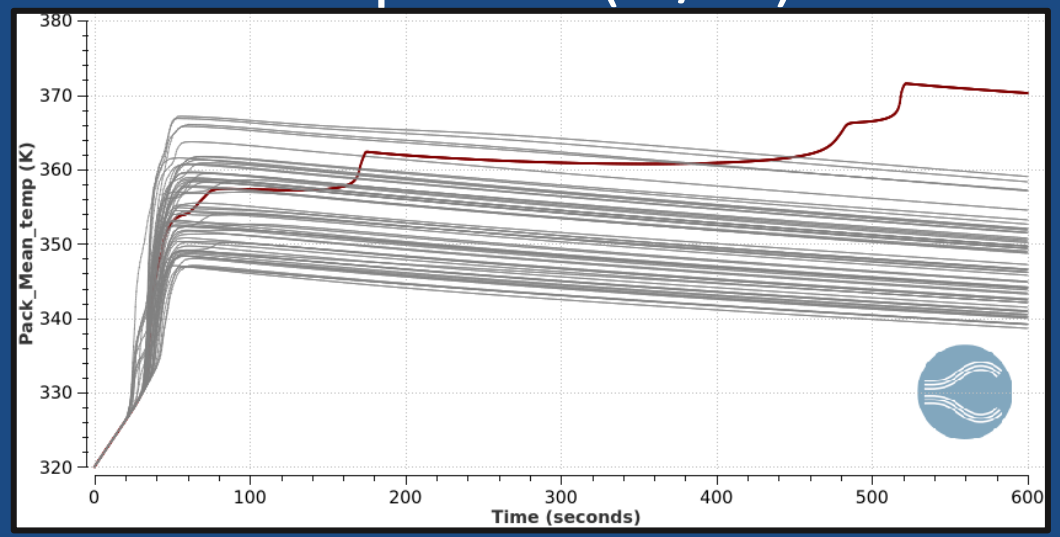
Triggered cell

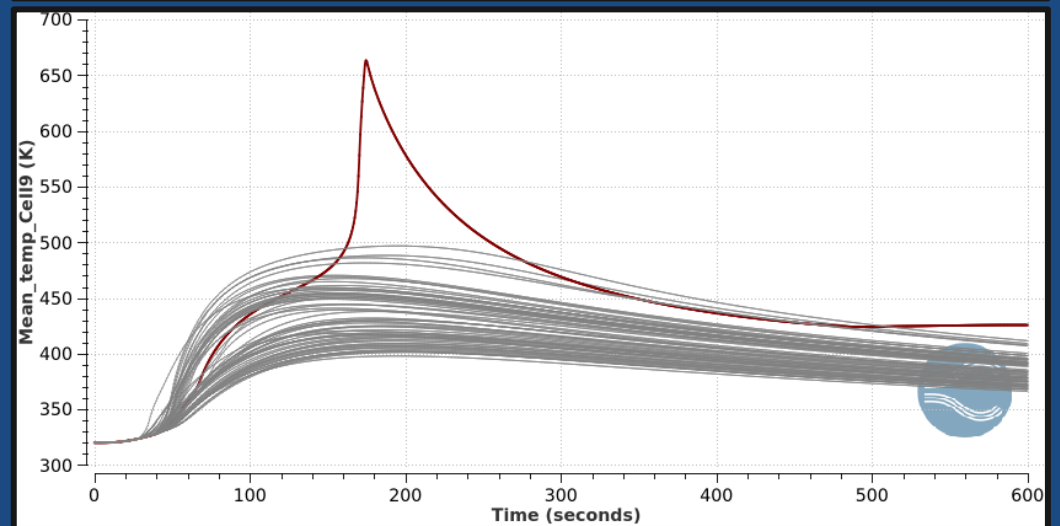
Statistical Studies of TR behaviour within pack (2/4)

31	32	33	34	35	36	37	38	39	40
21	22	23	24	25	26	27	28	29	30
11	12	13	14	15	16	17	18		
1	2	3	4	5	6	7	8	9	

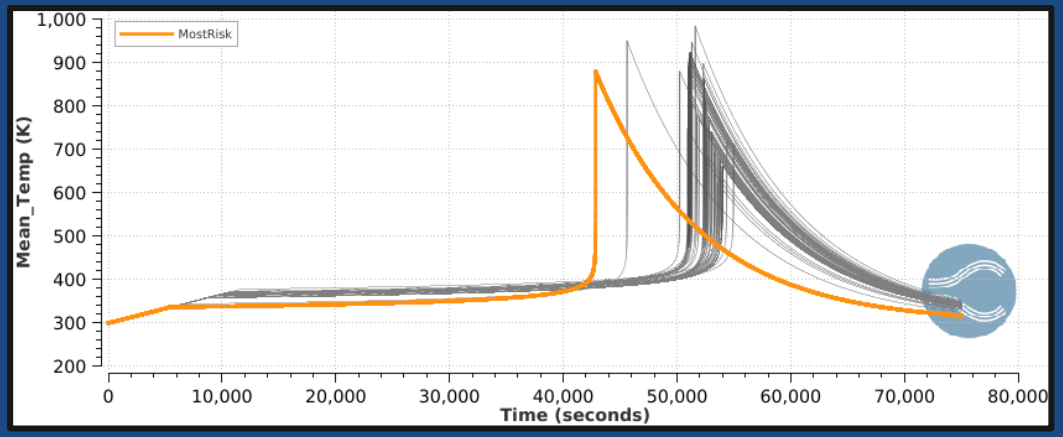


*60 cases

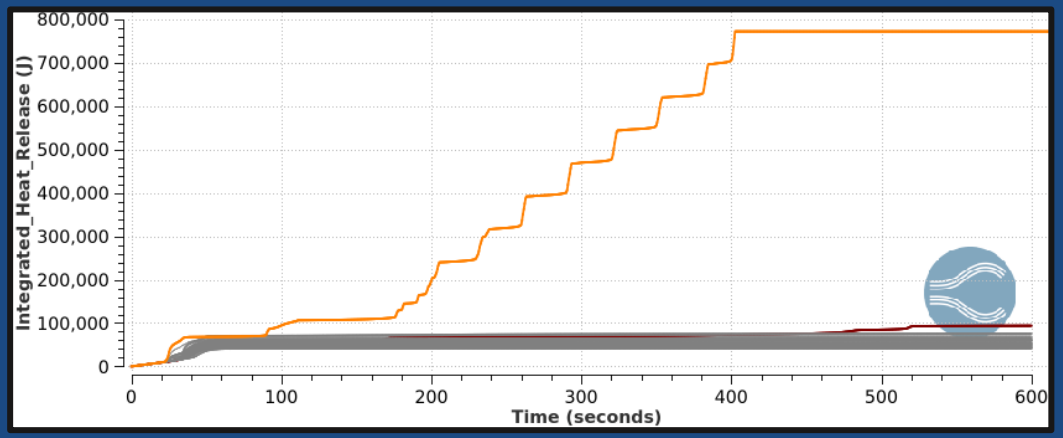


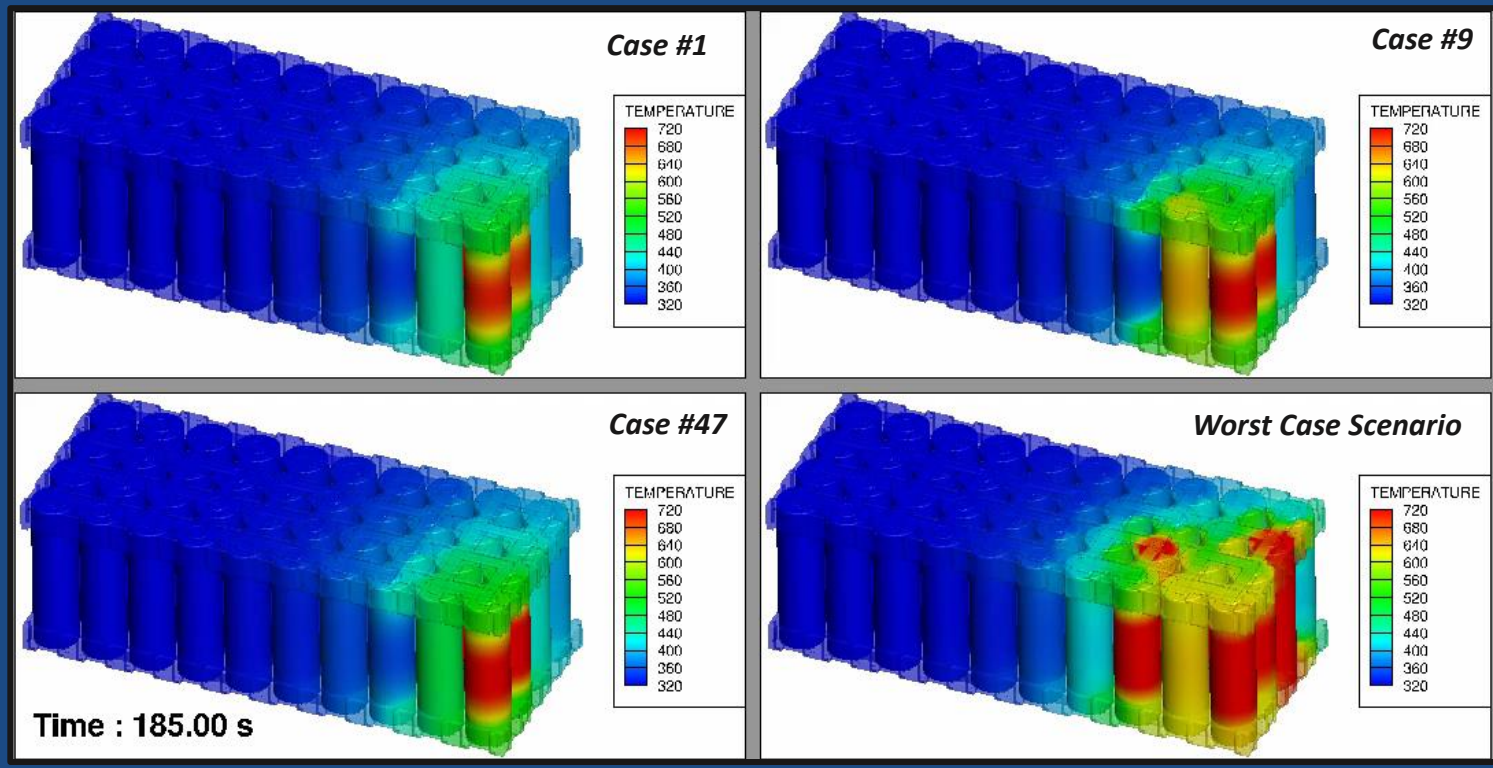


Statistical Studies of TR behaviour within pack (3/4)



Worst case scenario : All cells modeled with MostRisk parameters
Results in rapid TR propagation across entire battery pack





Triggered cell

Most Risk cell

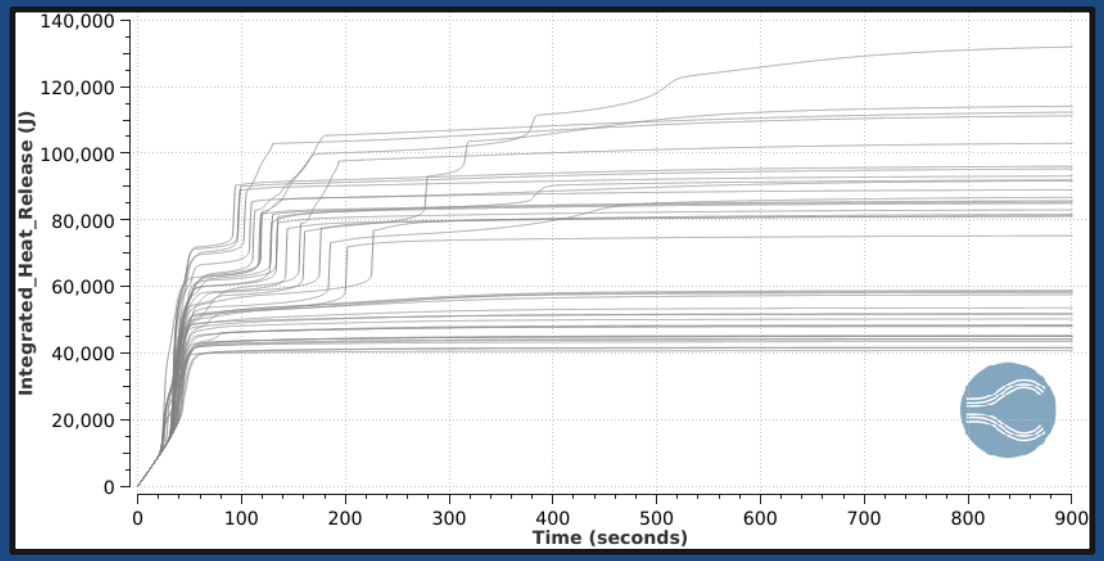
Statistical Studies of TR behaviour within pack (4/4)

31	32	33	34	35	36	37	38	39	40
21	22	23	24	25	26	27	28	29	30
11	12	13	14	15	16	17	18		
1	2	3	4	5	6	7	8	9	

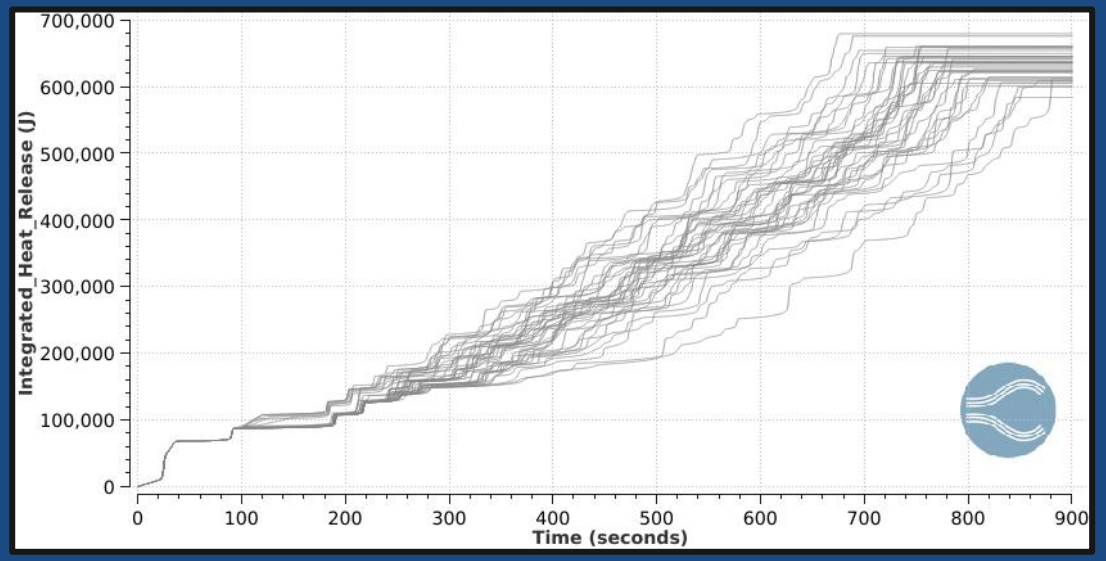
Multiple cases showcase TR in Cell9 and some in adjacent cells

31	32	33	34	35	36	37	38	39	40
21	22	23	24	25	26	27	28	29	30
11	12	13	14	15	16	17	18		
1	2	3	4	5	6	7	8	9	

TR propagation across the entire pack for 40/40 cases

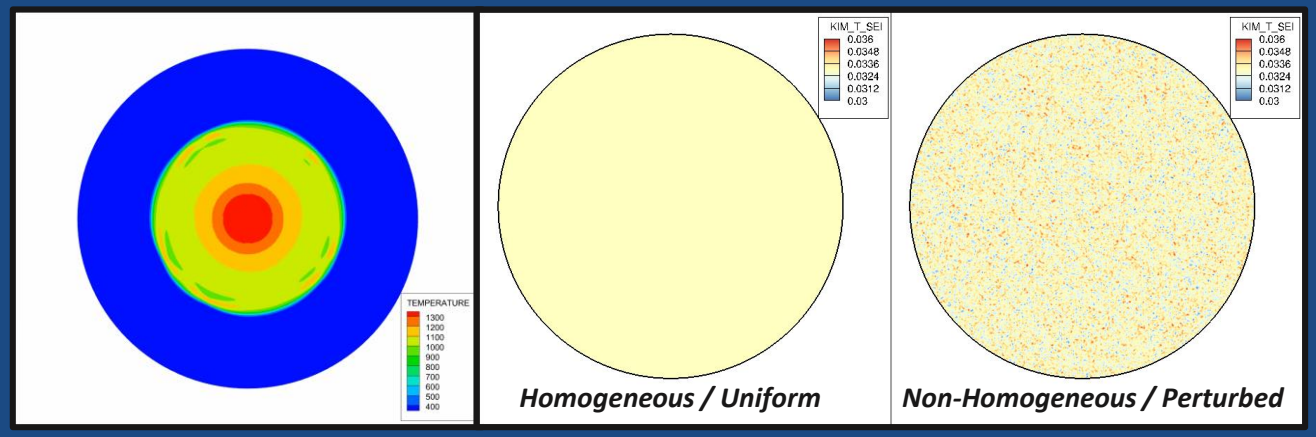


*40 cases



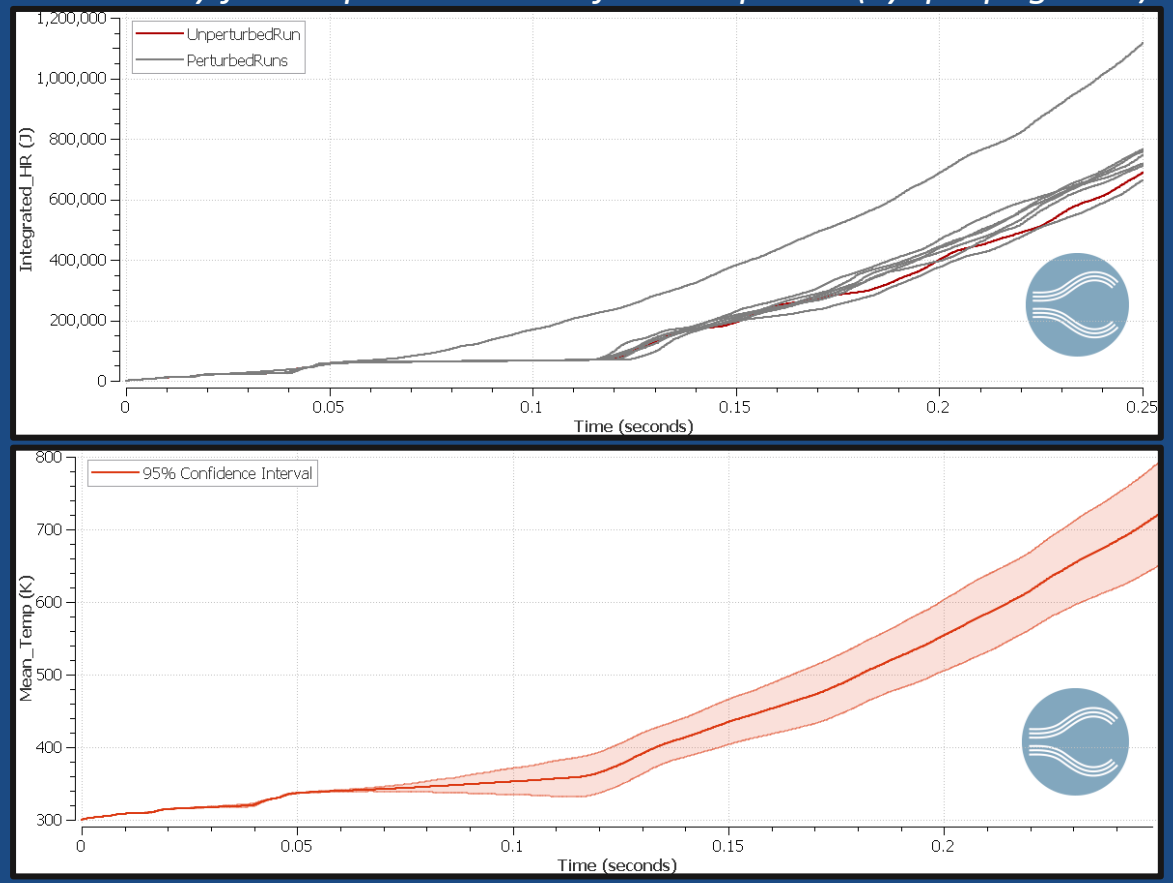
*40 cases

Species Perturbation Studies



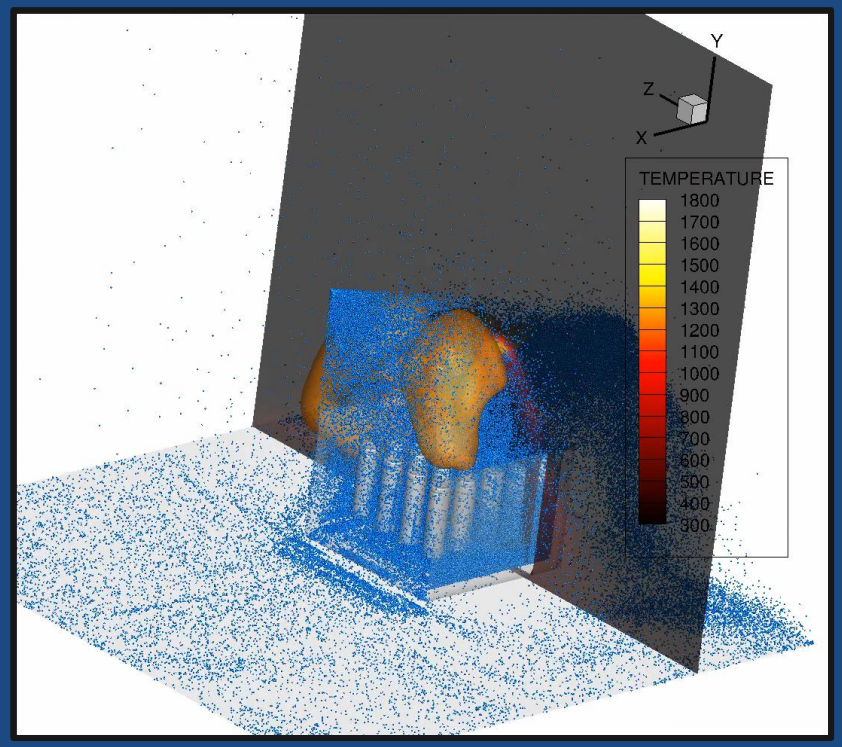
- Modeling propagation in a non-homogenous domain
  - Isotropic or Gaussian perturbations can be applied on the initial spatial distribution of any or all TR species
  - Differences arise after initial propagation, as expected
- Concurrent Perturbation Method can be utilized to obtain a confidence interval
  - N parallel runs with different random seed for perturbation
  - Cylindrical propagation showed high variability, outliers
  - Further investigations needed for complete understanding, esp on full 3D systems

CPM study for 1% perturbation of all TR species (cyl propagation)

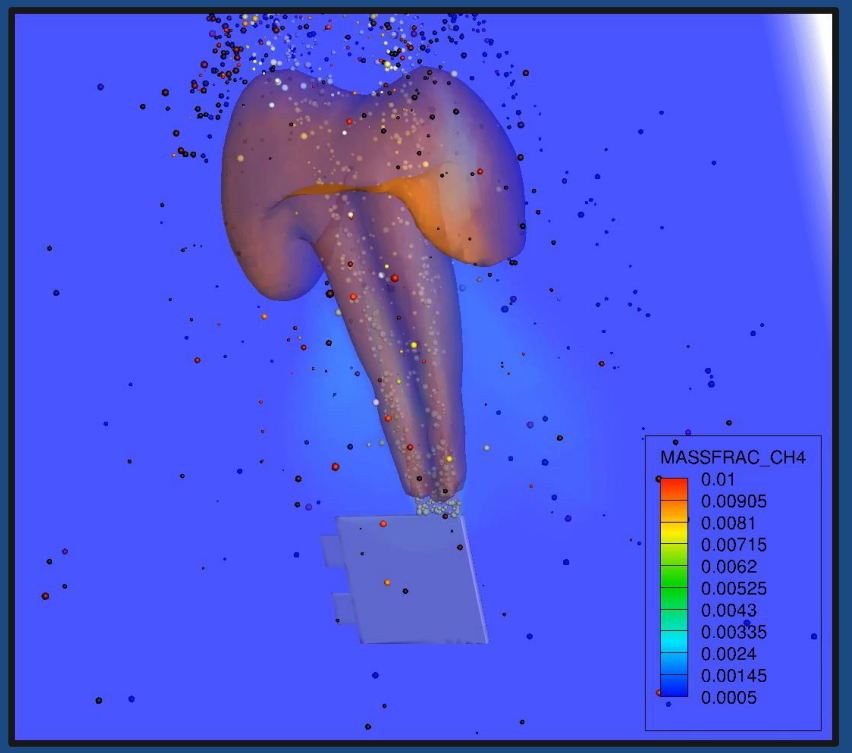


Lagrangian Particle Modeling within Battery simulations

Battery fire control



Vent gas ignition due to hot ejecta



THANK YOU!

CONVERGECFD.COM

Kislaya Srivastava,
Sr. Research Engineer, Convergent Science Inc.
kislaya.srivastava@convergecfd.com

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