CFD Modeling of Battery Thermal Runaway and Vent Gas Ignition Using Detailed Chemistry

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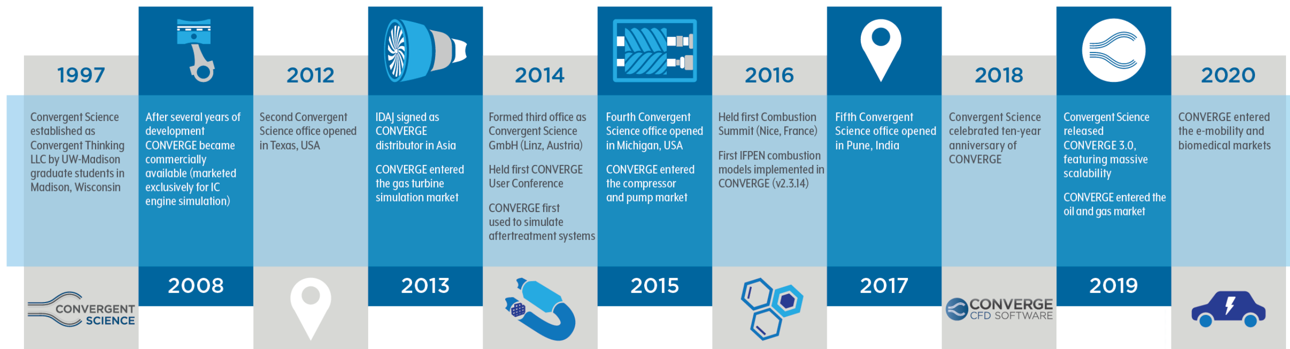
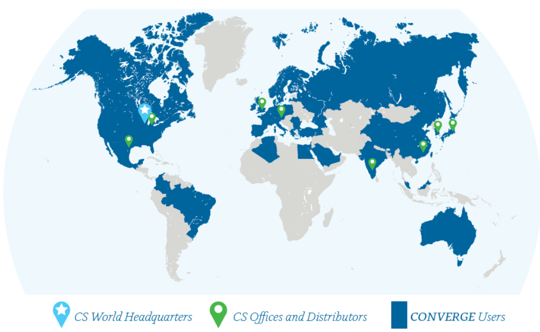
CONVERGE CFD SOFTWARE

Company Overview

- Convergent Science Inc. specializes in modeling turbulent reacting flows using CONVERGE CFD software
- 85% of engine manufacturers worldwide use CONVERGE

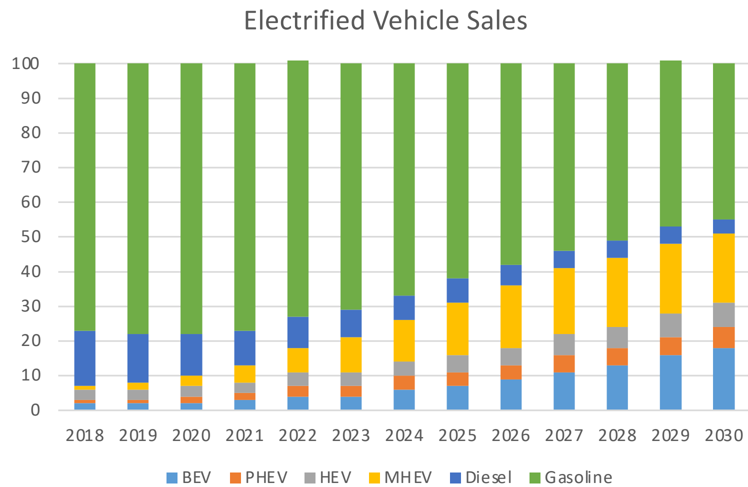
Convergent Science Inc. headquarters in Madison, Wisconsin





The Rise of Emobility

- Boston Consulting Group Sales Projections



- Electrified powertrains and internal combustion systems have an important role to play

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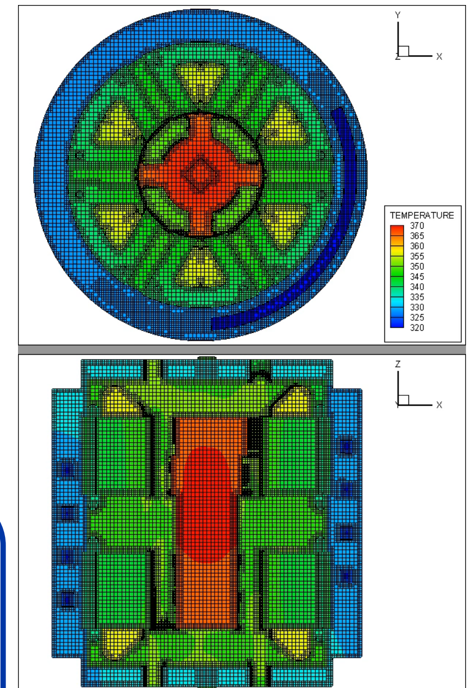
Primary Emobility Applications for CFD

- Batteries
  - Heat generation and cooling
    - Range of model fidelities for battery heat source specification
  - Thermal runaway
    - Simplified mechanisms reproduce experimental calorimetry data
  - Vent gas and ignition risk analysis
- Electric machines, *i.e.*, motors
  - Heat generation and cooling
    - Detailed electromagnetic loss calculations
- Power electronics
  - Heat generation and cooling
- Fuel cells
  - Water management and surface chemistry

CONVERGE CFD software is well-suited to simulations of 3D coupled flow, heat transfer, and chemistry in complex and/or moving geometries, with autonomous mesh generation and adaptive mesh refinement to reduce total time-to-solution.



Temperature distribution within an electric motor

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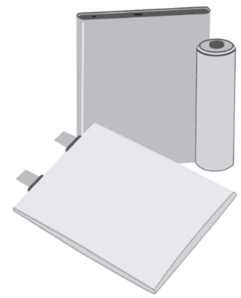
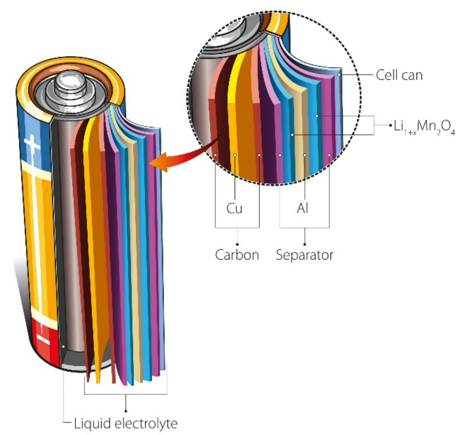
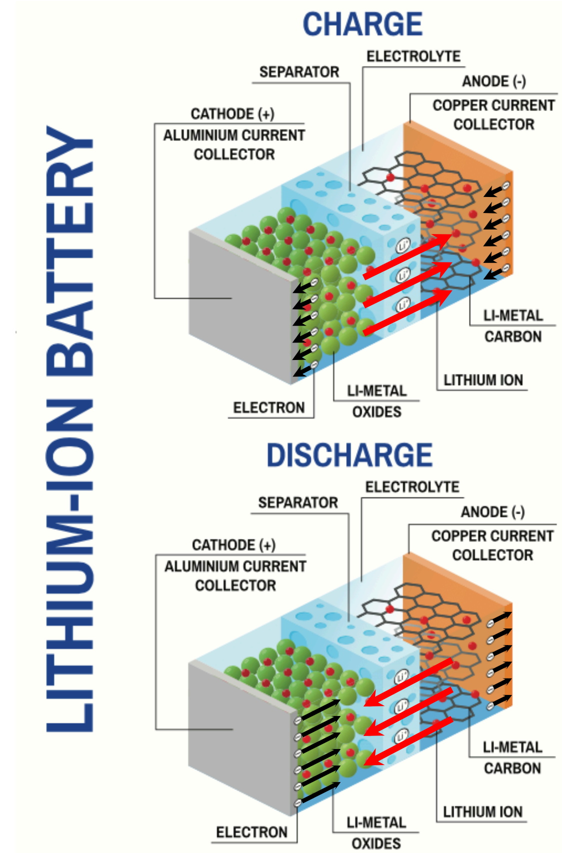
Lithium-Ion Battery Basics

- Battery cycle life is affected by many different stress factors including temperature, discharge current, charge current, and state of charge ranges
- Lithium-ion chemistry performs well at elevated temperatures but prolonged exposure to heat reduces battery life
- Thermal runaway risk begins around 80°C







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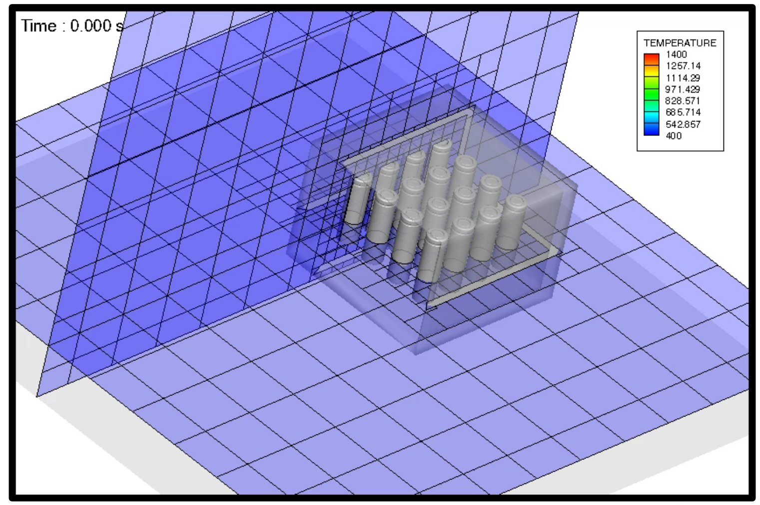
Thermal Failure of Pouch Cell

University of Texas Fire Research Group
https://www.utfireresearch.com/battery-fires



Detailed Chemistry

Detailed Chemistry

- CONVERGE contains the SAGE detailed chemical kinetics solver
- A reaction mechanism is a set of ***I*** elementary reactions between ***M*** species that describe an overall chemical reaction e.g. fuel oxidation

$$\sum_{m=1}^{M} \nu'_{m,i}\chi_m \rightleftharpoons \sum_{m=1}^{M} \nu''_{m,i}\chi_m \quad \text{for } i=1,2,\ldots.I \qquad \dot{\omega}_m = \sum_{i=1}^{I} \nu_{m,i} q_i \quad \text{for } m=1,2,\ldots.M \qquad \nu_{m,i} = \nu''_{m,i} - \nu'_{m,i}.$$

$$q_i = k_{i,f} \prod_{m=1}^{M} [X_m]^{\nu'_{m,i}} - k_{i,r} \prod_{m=1}^{M} [X_m]^{\nu''_{m,i}}. \qquad k_{i,f} = A_i T^{\beta_i} \exp\left(\frac{-E_i}{RT}\right),$$

- LLNL gasoline surrogate 1389 species, 5935 reactions
  - Reduced mechanism   48 species, 152 reactions

COMPUTATIONAL CHEMISTRY CONSORTIUM

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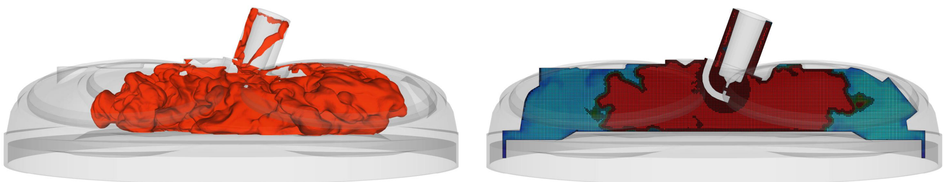
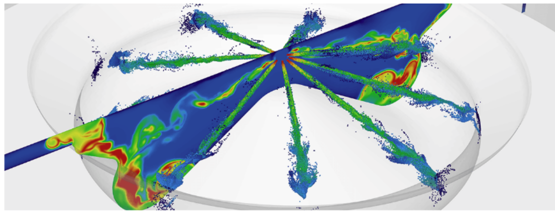
Common Detailed Chemistry Applications

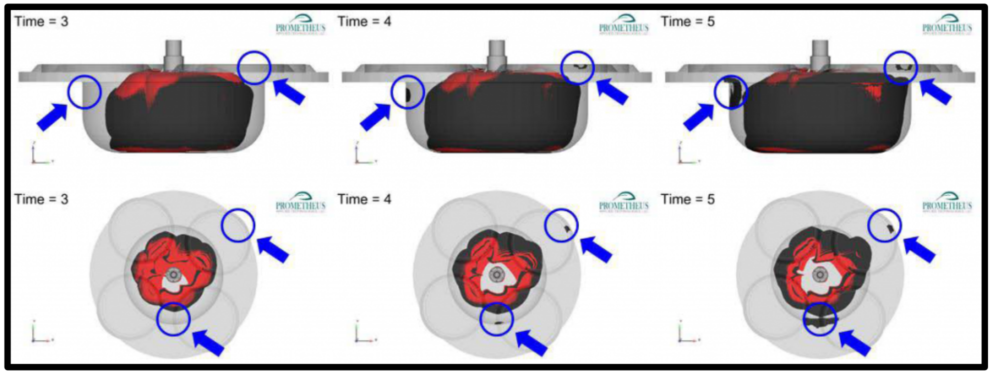
- Premixed Combustion



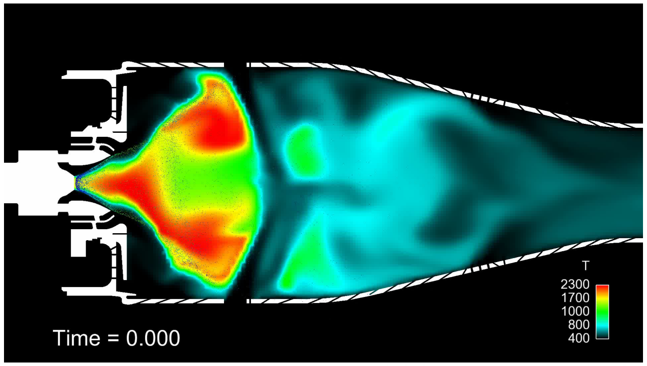
- Non-premixed Combustion



- Engine Knock



- Emissions

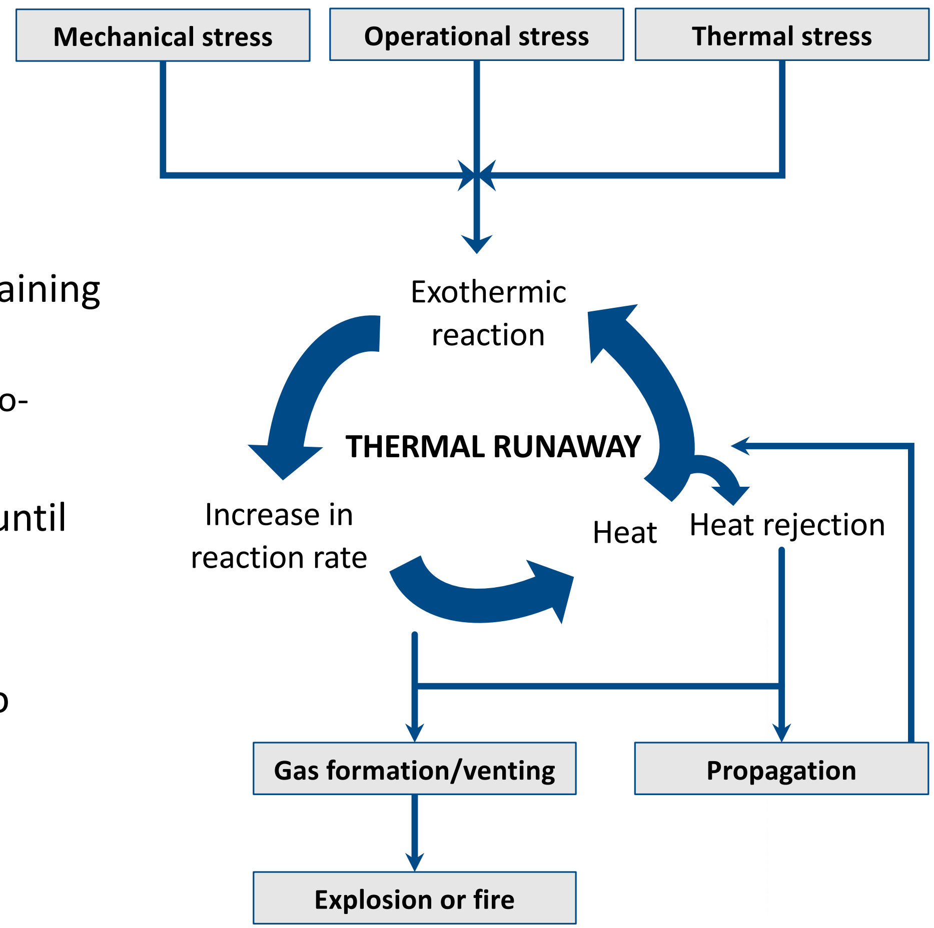


Courtesy of Prometheus Applied Technologies

Thermal Runaway

Thermal Runaway

- Exponential rise of cell temperatures due to self-sustaining exothermic reactions
  - Initiated due to mechanical, thermal, electrical, electro-chemical abuse
- Self-feeding heating rate within a cell that increases until the cell loses stability and ruptures
  - All thermal/electrochemical energy is released
- Risk: Critical failure, explosion or fires, propagation to adjacent cells in stack
- How can CFD help?
  - Thermal runaway predictions: Heat release, venting
  - Safety designs and cooling/fire suppression strategies



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Thermal Runaway Process Description

- Thermal runaway occurs when a cell has reached the point at which the temperature continues to increase on its own due to a number of exothermic reactions
  - 80°*C*: Solid electrolyte interphase (SEI) layer begins to decompose (reaction of lithium and electrolyte solvents)
  - 100°*C* – 120°*C*: Electrolyte begins to break down, generating gases within the cell e.g. CO_2, CO, CH_4, C_2H_6, C_2H_4, H_2
  - 120°*C* – 130°*C*: Separator melts allowing anode and cathode to make contact causing an internal short circuit
  - 130°*C* – 150°*C*: Cathode breaks down and releases oxygen
- Onset temperatures depend on individual battery chemistry

Warner, 2019

Kim Thermal Runaway Mechanism

- $LiCoO_2$/graphite battery
  - Also applied to $Li(Ni_{1/3}Co_{1/3}Mn_{1/3})O_2$/graphite battery by Zhang et al. (2020)
- 4 exothermic reactions
  - SEI decomposition (sei)
  - Anode and electrolyte (ne)
  - Cathode and electrolyte (pe)
  - Electrolyte decomposition (ele)
- CONVERGE detailed chemistry solver utilized to solve Arrhenius-style chemistry and calculate heat source
  - Premixed battery material combustion

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

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

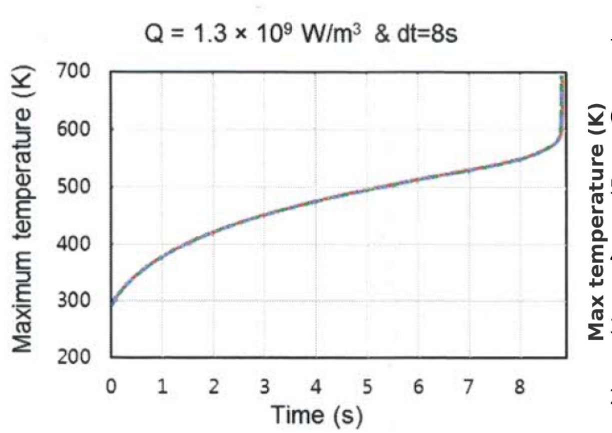
$$R_{pe}(T, \alpha, c_e) = A_{pe} \alpha^{m_{pe,p1}} (1-\alpha)^{m_{pe,p2}} \exp\left[-\frac{E_{a,pe}}{RT}\right]$$

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

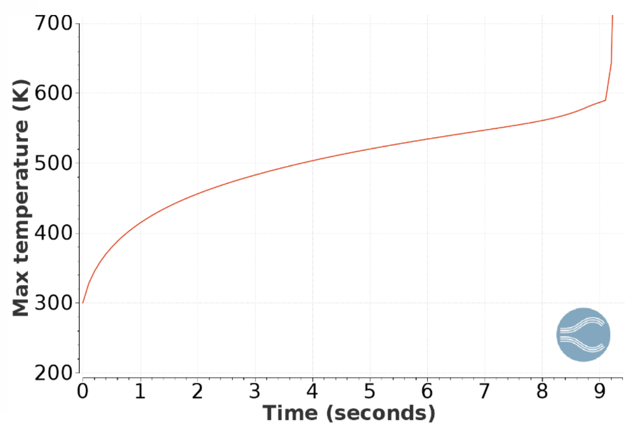
Kim et al., 2007

Kim Thermal Runaway Mechanism Validation

- Comparison to Zhang et al. (2020)
  - Prismatic cell with heat source due to battery damage



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

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Ren Thermal Runaway Mechanism

- $Li(Ni_{1/3}Co_{1/3}Mn_{1/3})O_2$/graphite battery
- 6 exothermic reactions
  - SEI film decomposition (SEI)
  - Anode and electrolyte (An-E)
  - Anode and binder (An-B)
  - Cathode (O2) and anode (Cat-An)
  - Cathode (O2) and binder (Cat-B)
  - Cathode decomposition (Cat)
- Differential scanning calorimetry (DSC) results provide pre-exponential factors, activation energies, and mechanism functions

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

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

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

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

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

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

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

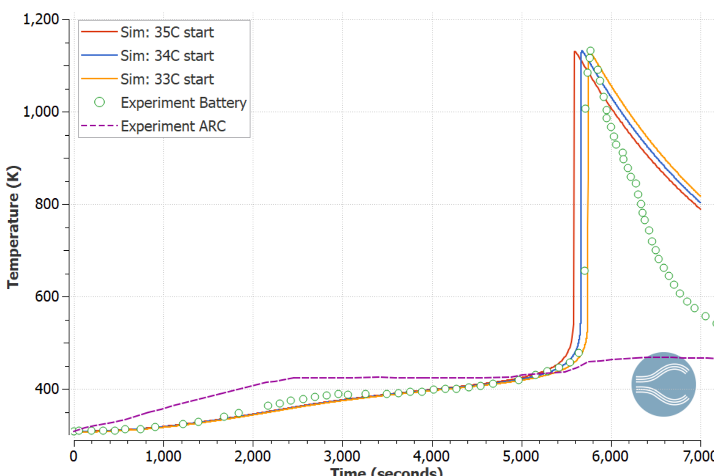
$$c_{Cat} = 1 - \int \kappa_{Cat} dt$$

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

Ren et al., 2018

Thermal Runaway Mechanism Validation (Easy)

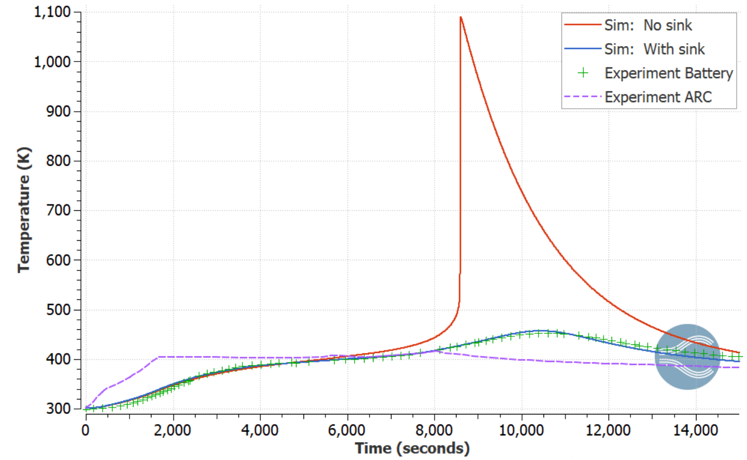
- 150°C Ren et al. Case
  - Pouch cells in an accelerated rate calorimeter (ARC)
  - Simulation runs in less than a minute
    - Lumped analysis, T_{ARC} extracted from line plots

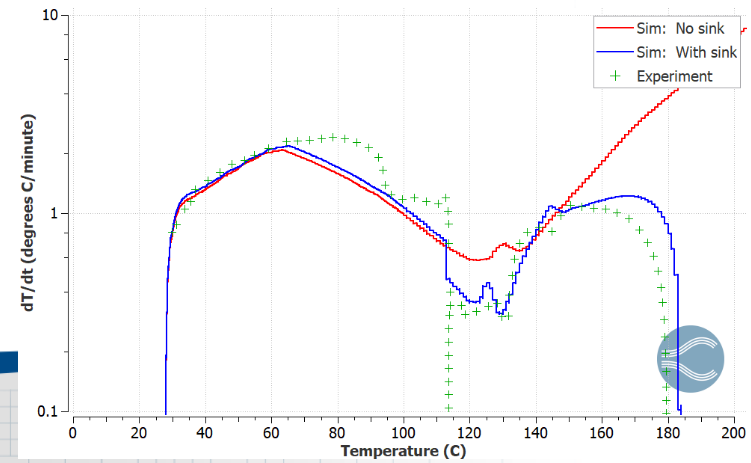


Ren et al., 2018

Thermal Runaway Mechanism Validation (Hard)

- 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



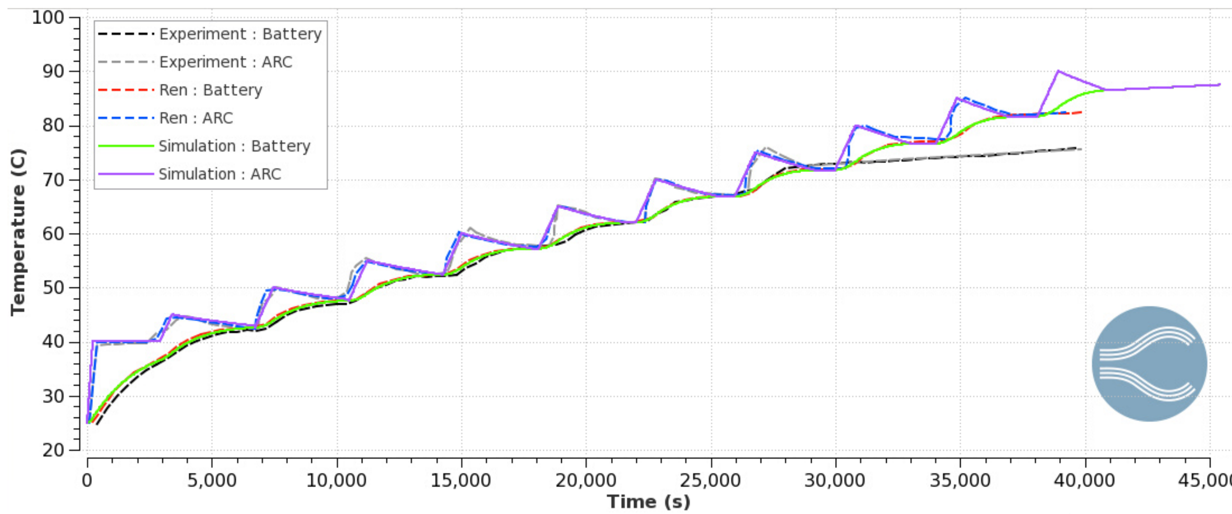


Ren et al., 2018

Self-Heating Onset Validation

- Adiabatic Thermal Runaway Ren et al. Case
  - 0.01 °*C* per minute

	T_{onset} °*C*
Experiment	72.39
Ren Model	81.44
CONVERGE Model	86.48

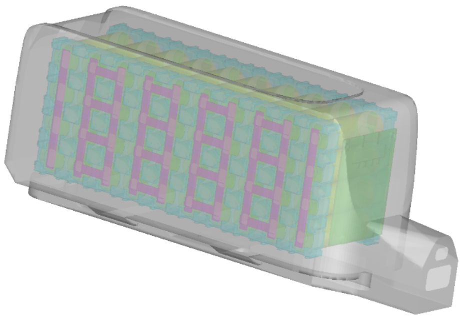


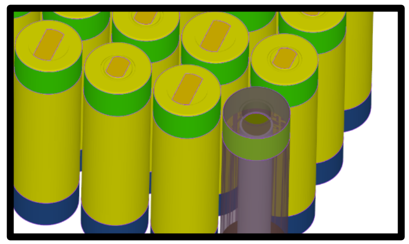
Ren et al., 2018

Vent Gas Analysis

Electric Bike Battery Vent Analysis

- Individual cylindrical battery cell selected to introduce vent gas





- Vent gas composition from experimental measurements

Cell	SOC	mmol	H_2%	CO_2%	CO%	CH_4%	C_2H_4%	C_2H_6%
NCA	25	67	15.5	62.7	5.5	8.7	7.5	
NCA	50	157	17.5	33.8	39.9	5.2	3.2	0.4
NCA	100	314	26.1	17.5	44	8.9	2.7	0.9
LFP	100	32	29.4	48.3	9.1	5.4	6.3	0.5

Golubkov et al., 2015

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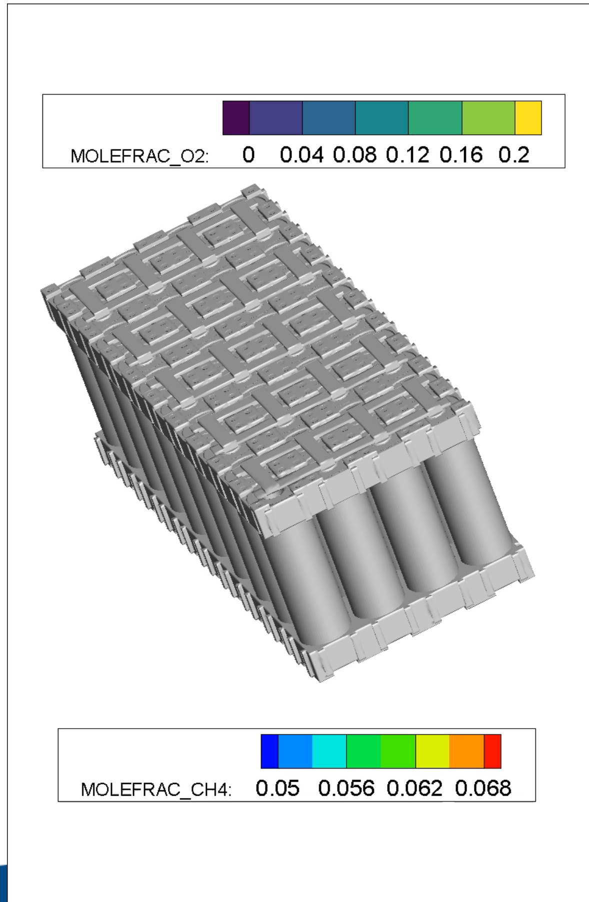
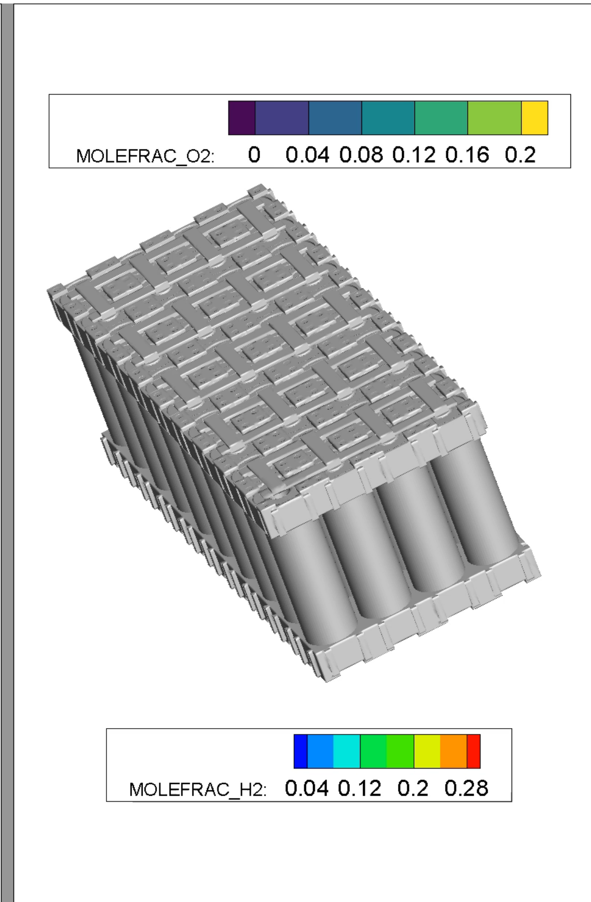
Flammability Limits

- CH_4 mole fractions
  - LEL 0.05
  - UEL 0.15
  - 0.094 Stoich.
- Isosurfaces
  - 0.05 CH_4
  - 0.06 CH_4
  - 0.10 O_2
  - 0.2 O_2





- H_2 mole fractions
  - LEL 0.04
  - UEL 0.75
  - 0.294 Stoich.
- Isosurfaces
  - 0.04 H_2
  - 0.20 H_2
  - 0.02 O_2
  - 0.2 O_2

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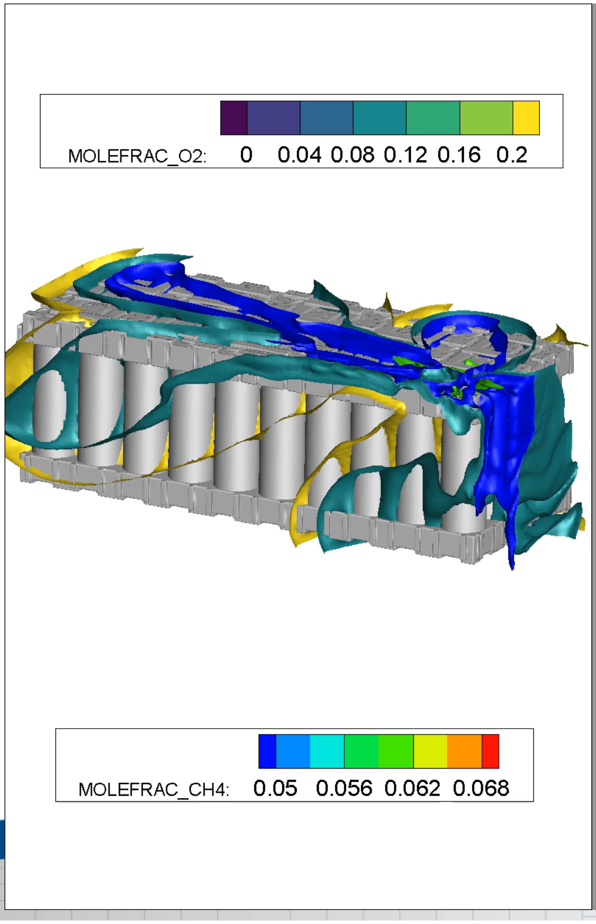
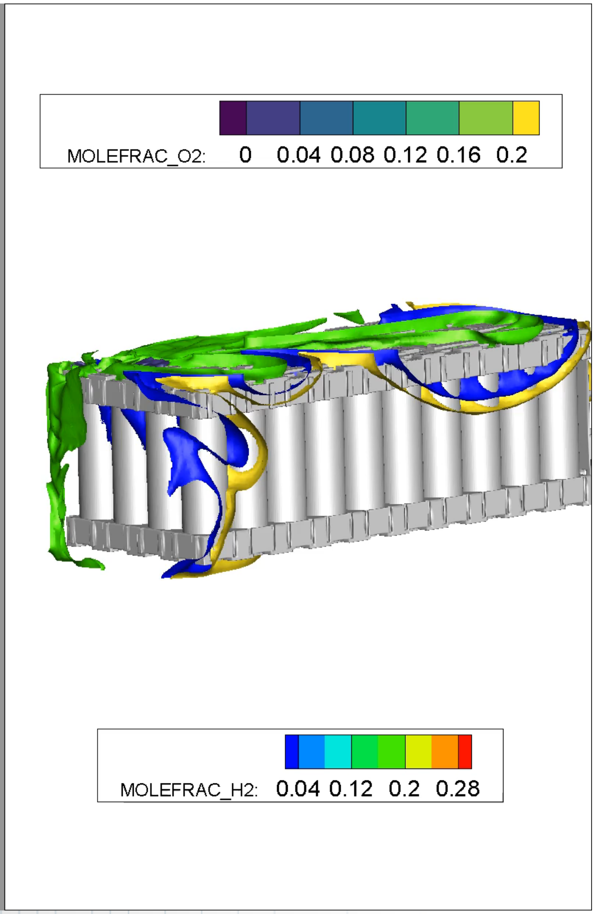
Intra-Pack Combustion

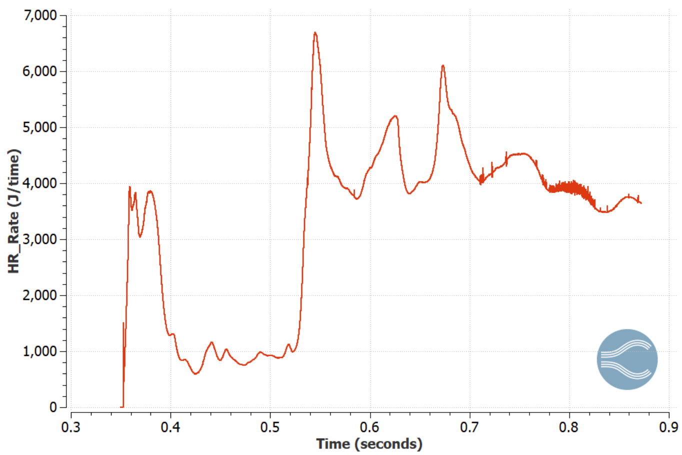
- Combustion Energy Release
  - 0.22 g of vent gas over 0.5 s
    - 7 g over 10 s for complete vent
    - 0.016 g H_2 and CH_4 combined
  - 227 J released inside pack over 0.15 s
    - 1273.7 J available in H_2 and CH_4 combined
  - 1.03 MJ/kg-vent gas
- Thermal Runaway Energy Release
  - 900000 J from 1.1 kg battery
  - 0.818 MJ/kg-battery

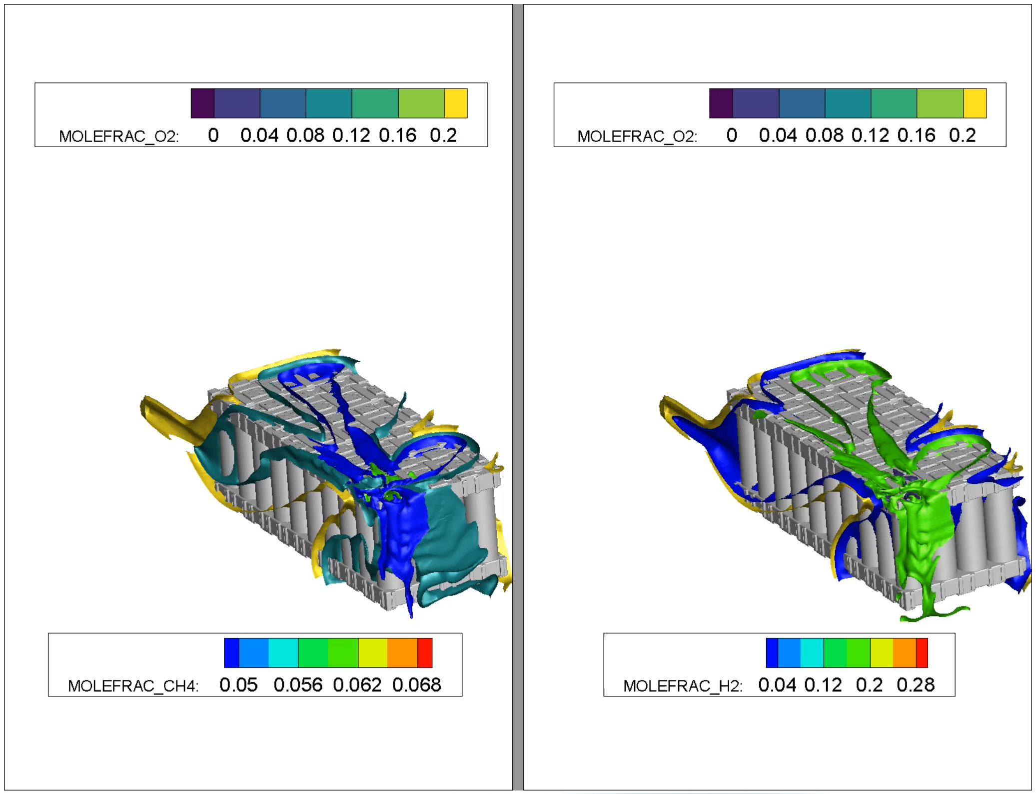




For Best Results, Add Oxygen

- Combustion Energy Release
  - 0.59 g of vent gas over 0.87 s
  - 1482 J released outside pack over 0.37 s





Thermal Runaway Propagation

Google Search: Electric Bike Battery Pack Fires

Why Do E-Bikes Catch Fire?

LYFT SUSPENDED E-BIKE SERVICE IN SAN FRANCISCO FOLLOWING FOUR BATTERY FIRES. THEN, A LIME E-BIKE CAUGHT FIRE IN SEATTLE. WE INVESTIGATED THE REASONS WHY ELECTRIC BIKE LITHIUM-ION BATTERIES BURN UP.

BY DAN ROE Aug 23, 2019

https://www.bicycling.com/bikes-gear/a28778383/electric-bike-explosion/

BATTERY FIRES CREATE CONCERNS FOR EVERY ELECTRIC BIKE OWNER (UPDATED)

July 20, 2020 jimmymac

http://jimmymacontwowheels.com/battery-fires-create-concerns-for-every-electric-bike-owner/

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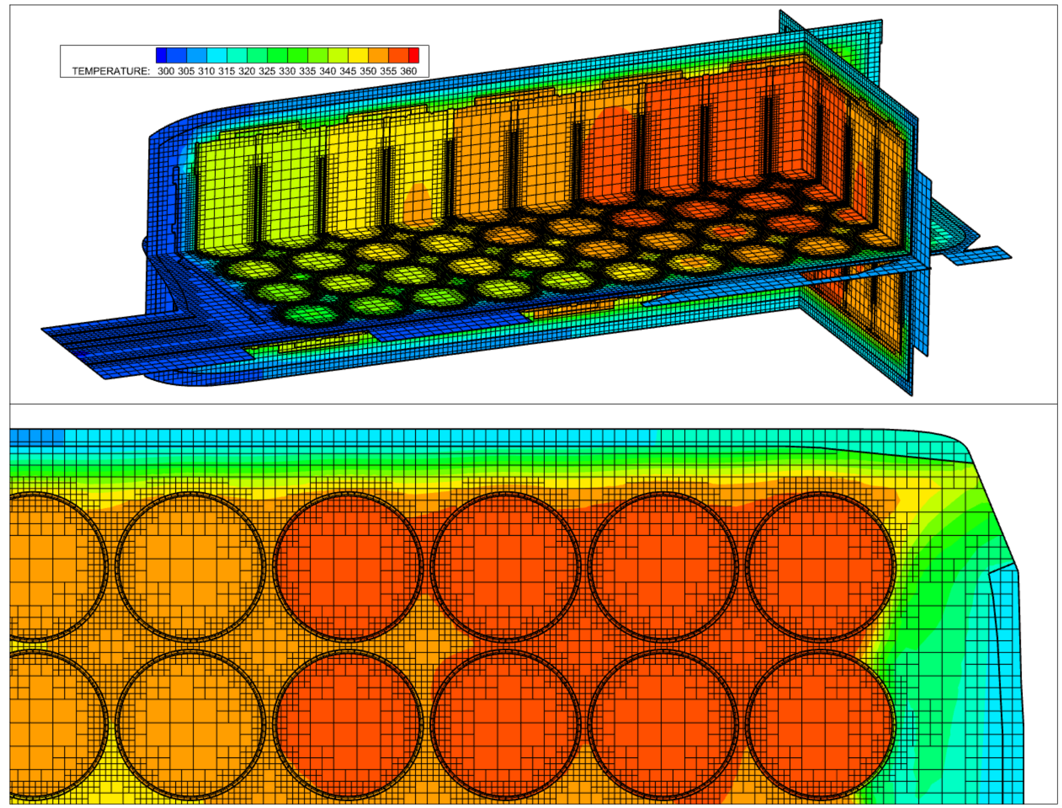
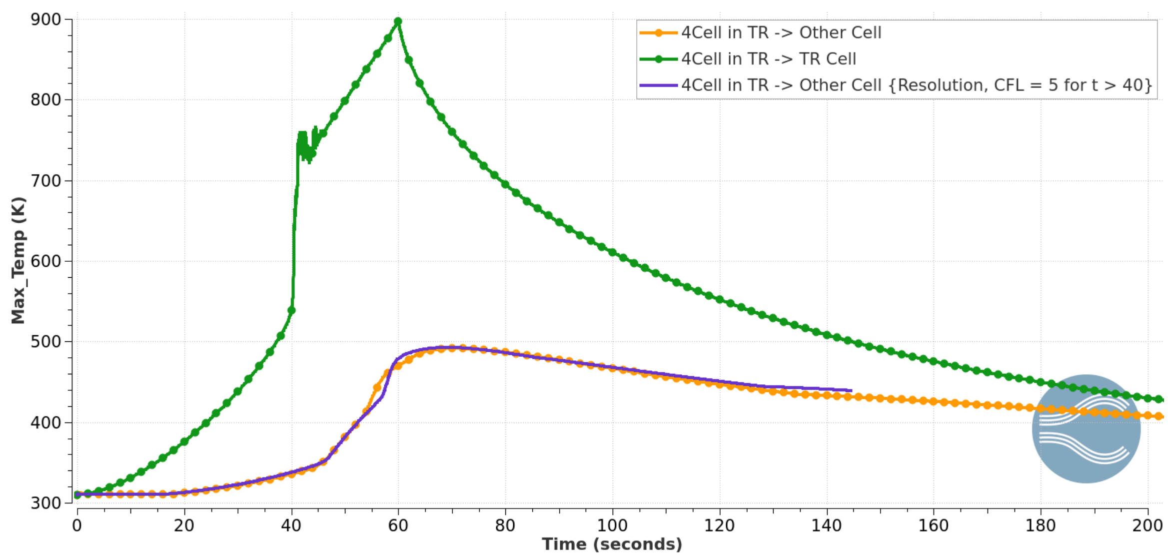
Warm-up Simulation

- Steady-state simulation
  - 2 W internal heat generation per cell (1C)
  - 5 m/s air mass flow rate at 300 K
  - Conjugate heat transfer solution couples temperature solution in fluid and solids:
    - Frame
    - Frame mount
    - Spacers
    - Cells
    - Nickel strips
    - BMS



Thermal Runaway Simulation

- Transient simulation
  - 4 cells experience 200 W elevated internal heat generation
  - No propagation
    - Maximum temperature is high, but not mean temperature



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Future Work

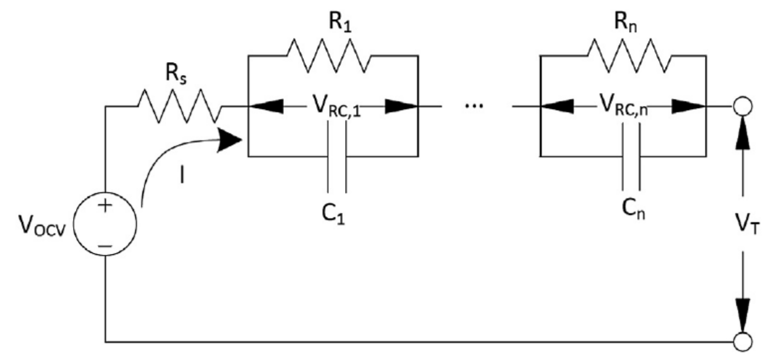
- Combine battery electrical network equivalent heat source (v3.1) with thermal runaway mechanisms

Terminal voltage: $$V_T = V_{OCV} - IR_S - \sum_{i=1}^{n} V_{RC,i}$$

$$\frac{dV_{RC,i}}{dt} = -\frac{1}{R_i C_i} V_{RC,i} + \frac{1}{C_i} I$$

$$\frac{dSOC}{dt} = -\frac{1}{C_{bat}} I$$

$$Q = I(V_{OCV} - V_T)$$



Lin et al., 2014

- Investigate thermal runaway propagation via vent gas combustion

THANK YOU!

CONVERGECFD.COM

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