Experiments and Numerical Modeling of Fires Associated with Lithium-Ion Batteries Thermal Runaway

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Research Institutes

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- Environmental chamber from ***NASA GRC***.
- High Performance Computing Cluster at CWRU.

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http://engineering.case.edu/groups/CFDLab/

Lab Mission:

- To continue to improve the accuracy and realism of the chemistry and physics underlying *computational models* of combustion, fire, and fire behavior.
- To design/perform *normo- and micro- gravity experiments* that provide data that can help clarify, prove, or suggest fire models.

Research Interests:
Fire modeling, material flammability, solid pyrolysis, ignition and flame spread, microgravity combustion, wildland fire, battery fire.

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Lithium-Ion Battery (LIB) Fires

Samsung Galaxy Note 7 Explosion (2016). Picture courtesy of New York Time.

A Tesla Model S fire after crash (2018) [NTSB/SR-20/01, 2020]

Fire of ESS in a renewable energy facility in South Korea (2018) [Park et al, Fire Sci. Engr., 2018]

A Tesla Model S was in a junkyard for 3 weeks and suddenly burst into flames. Picture courtesy of The Washington Post.

- Fire incidents related to lithium-ion batteries are more and more frequent.
- The global demand for battery cells is expected to double from 725 GWh in 2020 to 1500 GWh in 2030 [Duffner et al., 2021].

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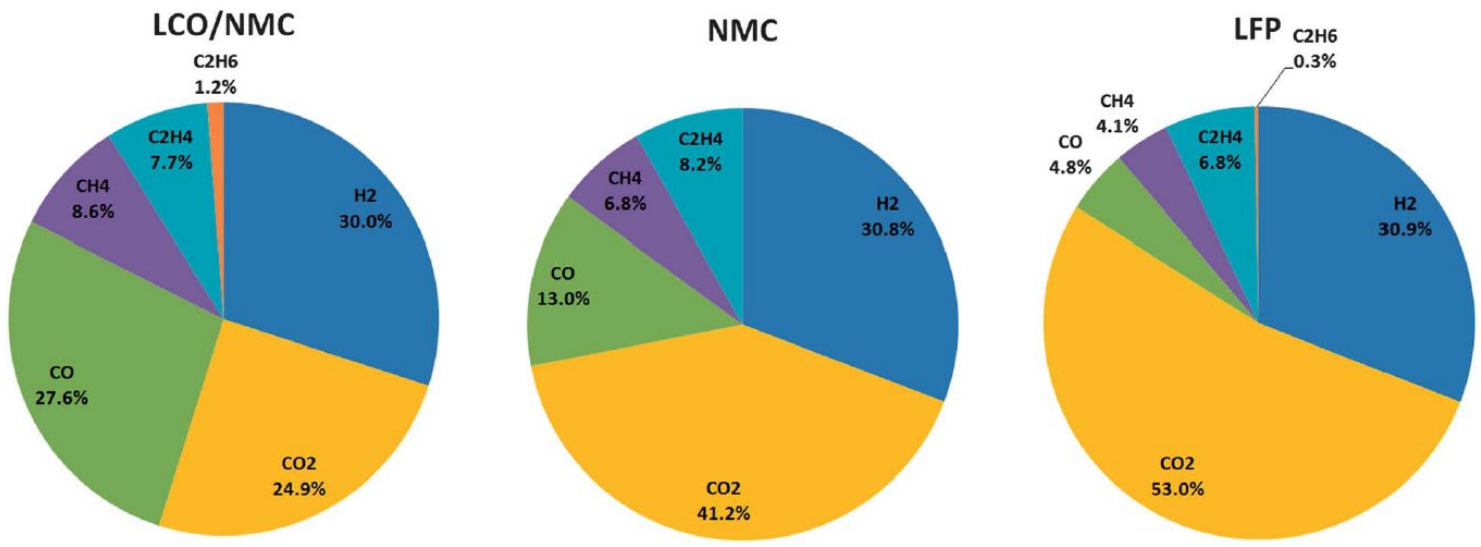
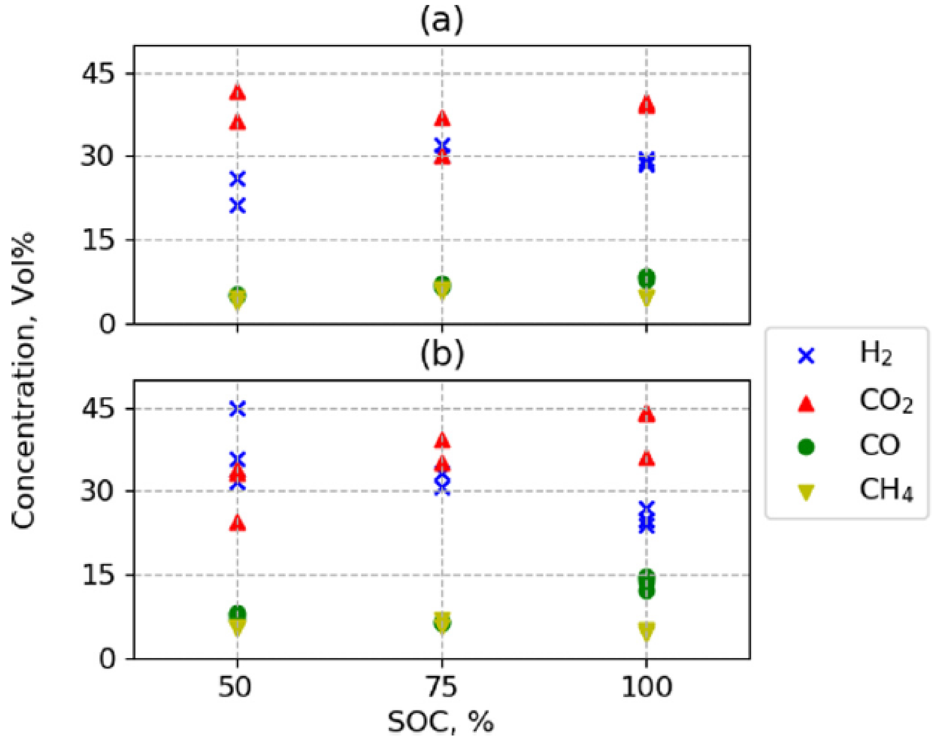
Flammable Venting Gases



Gas release from 18650 cells thermal runaway in Argon
[Golubkov et al., The Royal Society of Chemistry, 2014]



Gas release from 10 Ah pouch (a) 10 Ah single cell, (b) 10 Ah array in Nitrogen.
[Kennedy et al., Journal of Power Sources, 2021]

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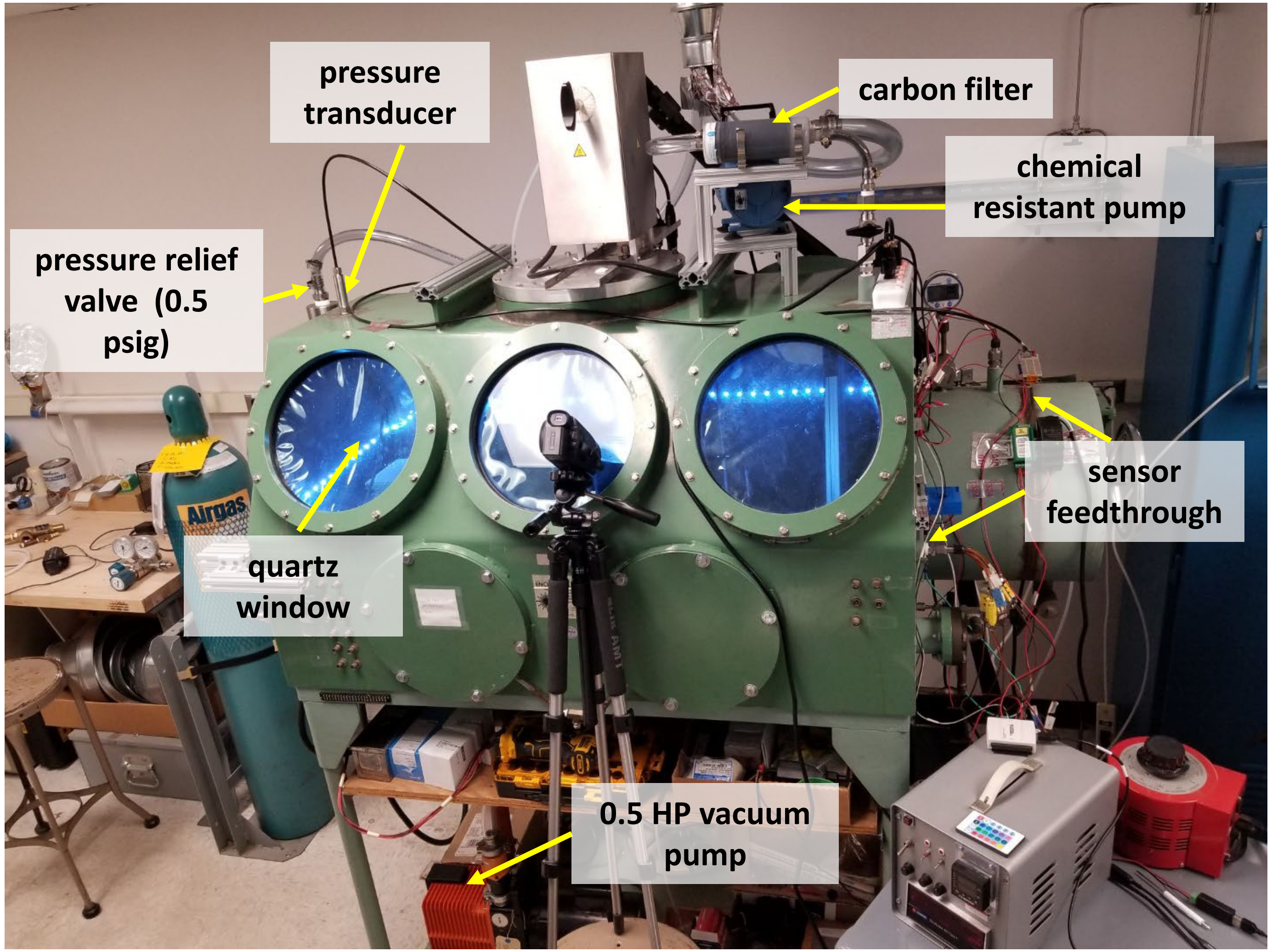
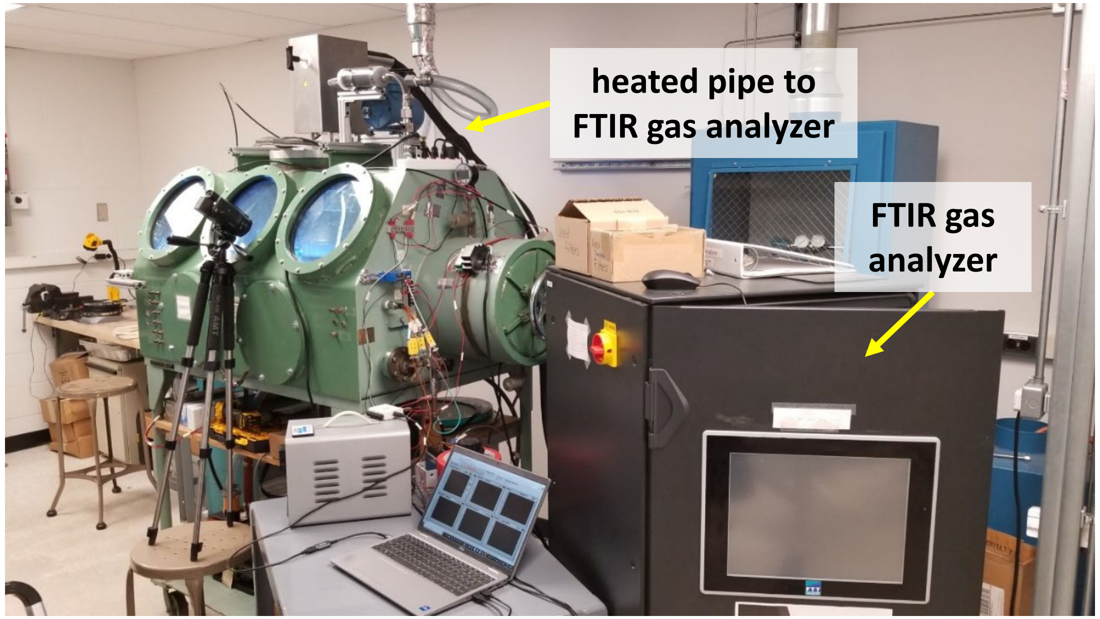
Objectives

- Perform ***experiments*** to investigate the LIB thermal runaway and its subsequent fires.
- Obtain parameters that are needed to construct a ***numerical model*** for the LIB fires.
- Develop a numerical model to study fire ***propagation*** between cells and to understand the ***scalability*** of battery fire.

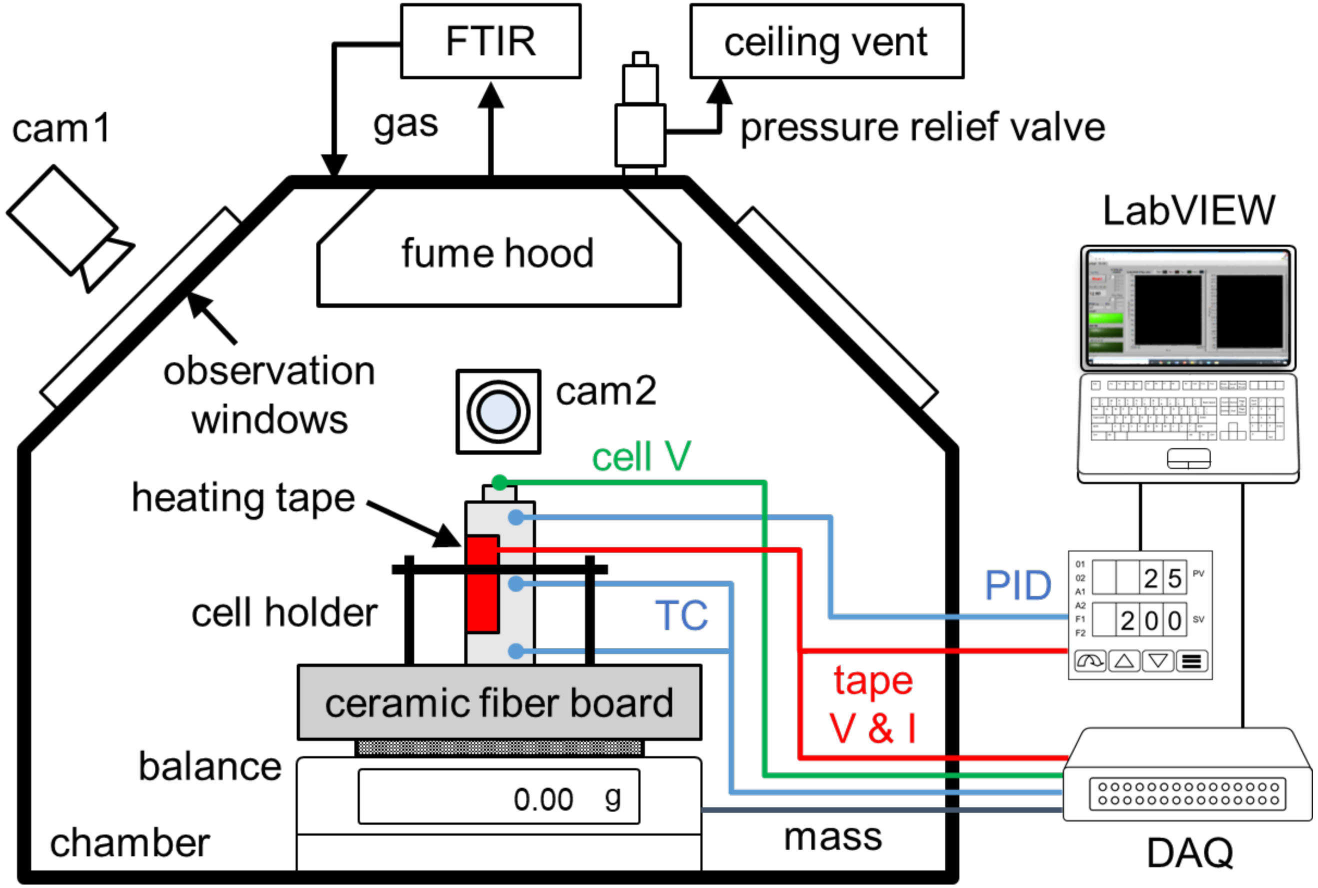
Experiment Apparatus





- Chamber volume ~ 600L.
- The FTIR detects 21 gas species: H_2O, CO_2, CO, NO, NO_2, N_2O, SO_2, HCl, HCN, HBr, HF, NH_3, C_2H_4, C_2H_6, C_3H_8, C_6H_{14}, CH_4, HCHO, C_6H_6O, C_3H_4O, and COF_2.

Schematics of the Experiment Setup



- PID controlled heating tape (cell heating rate: 10 °C/min).
- K-type thermocouples on cell surface.
- Mass balance (0.1 g precision).
- Cell voltage measurement.
- Front and side video recorders.
- FTIR gas analyzer (21 gas species).
- H_2 sensor (in progress).

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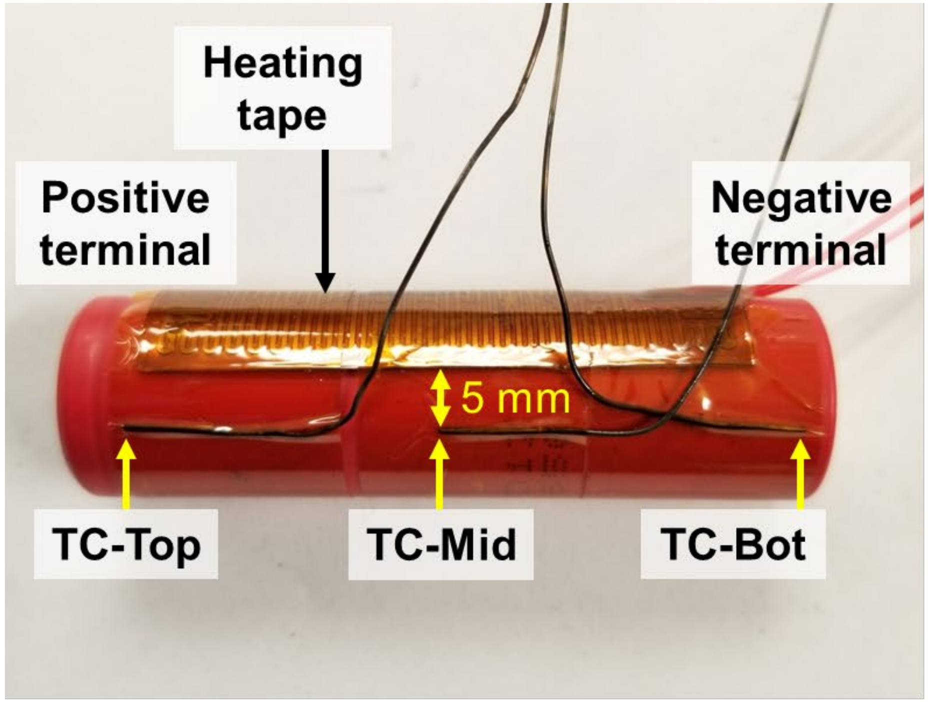
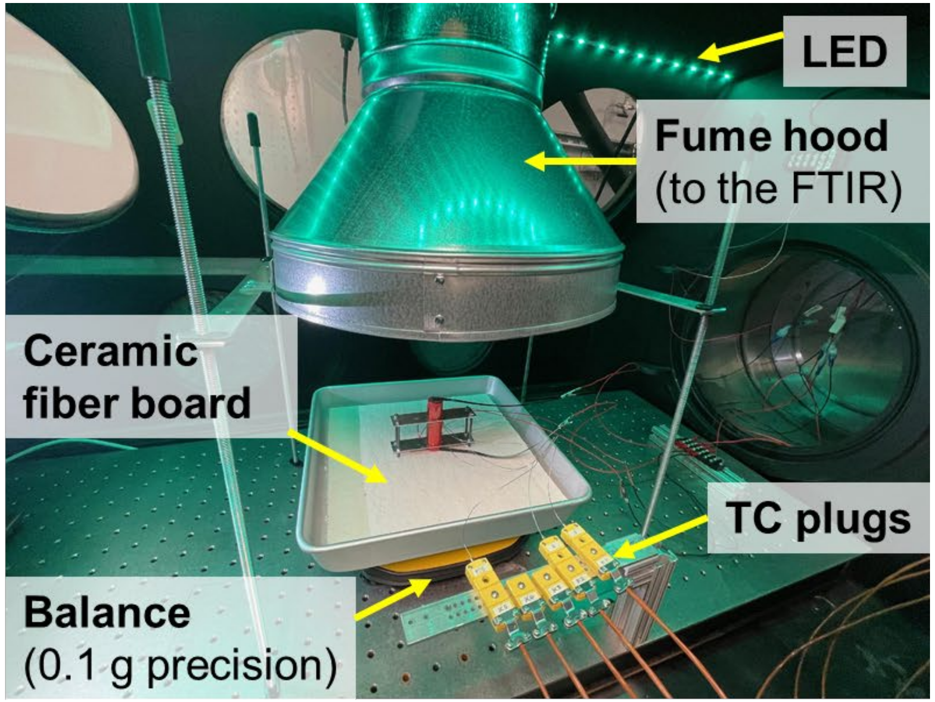
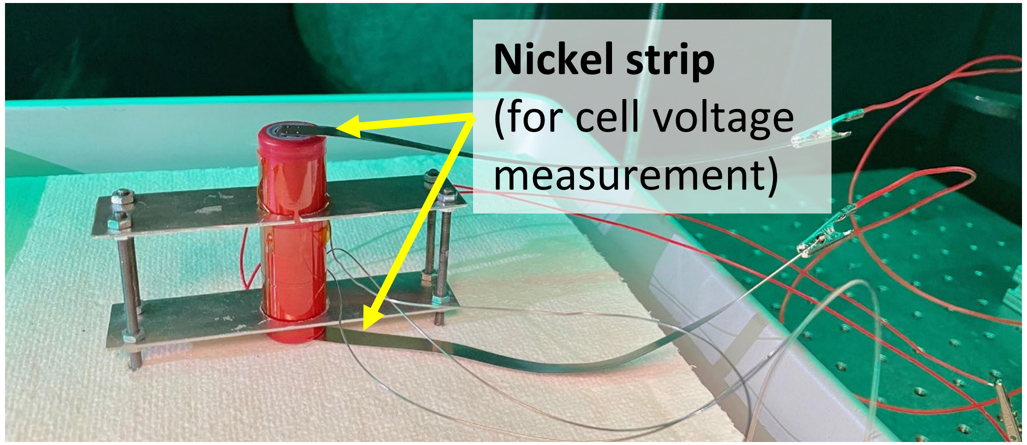
Cylindrical Cell Setup







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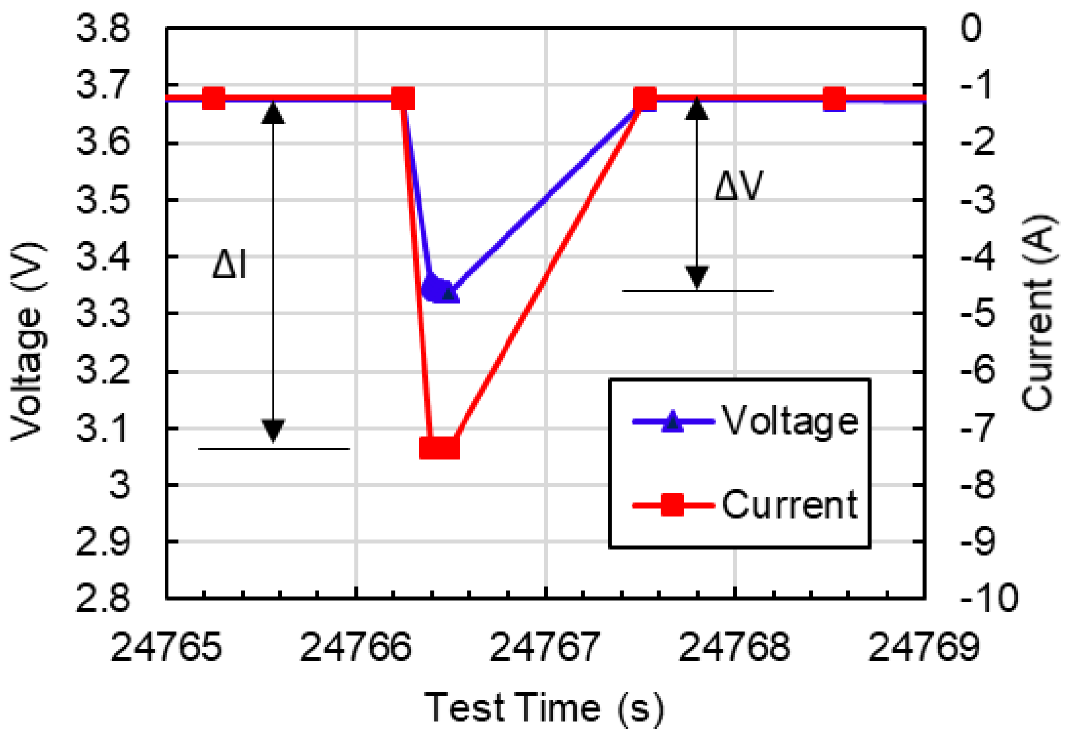
Cell Conditioning



All battery experiments were conducted within <u>24 hours</u> since the cell conditioning.

Step 1: Rest 30s

Step 2: Charge: 1.3A to 4.2V, 4.2V until current falls to 130mA

Step 3: Rest 30s

Step 4: Discharge:

- 4-1: 1.3A for 3599s (Sampling rate: 0.1 Hz)
- 4-2: 1.3A for 1s (to 50% SOC) (Sampling rate: 100 Hz)
- 4-3: Internal resistance measurement: Current pulse under -3C (-7.8 A) for 100 ms (sampling rate: 100Hz)
- 4-4: 1.3A for 1s. (Sampling rate: 100 Hz)
- 4-5: 1.3A to 2.7V (Sample rate: 0.1 Hz)

Step 5: Rest 30s

Repeat steps 1-5

Step 6: Charge: 1.3A to 4.2V, 4.2V until current falls to 130mA

Step 7: Rest 30s

Step 8: Discharge: 1.3 A to the desired SOC.

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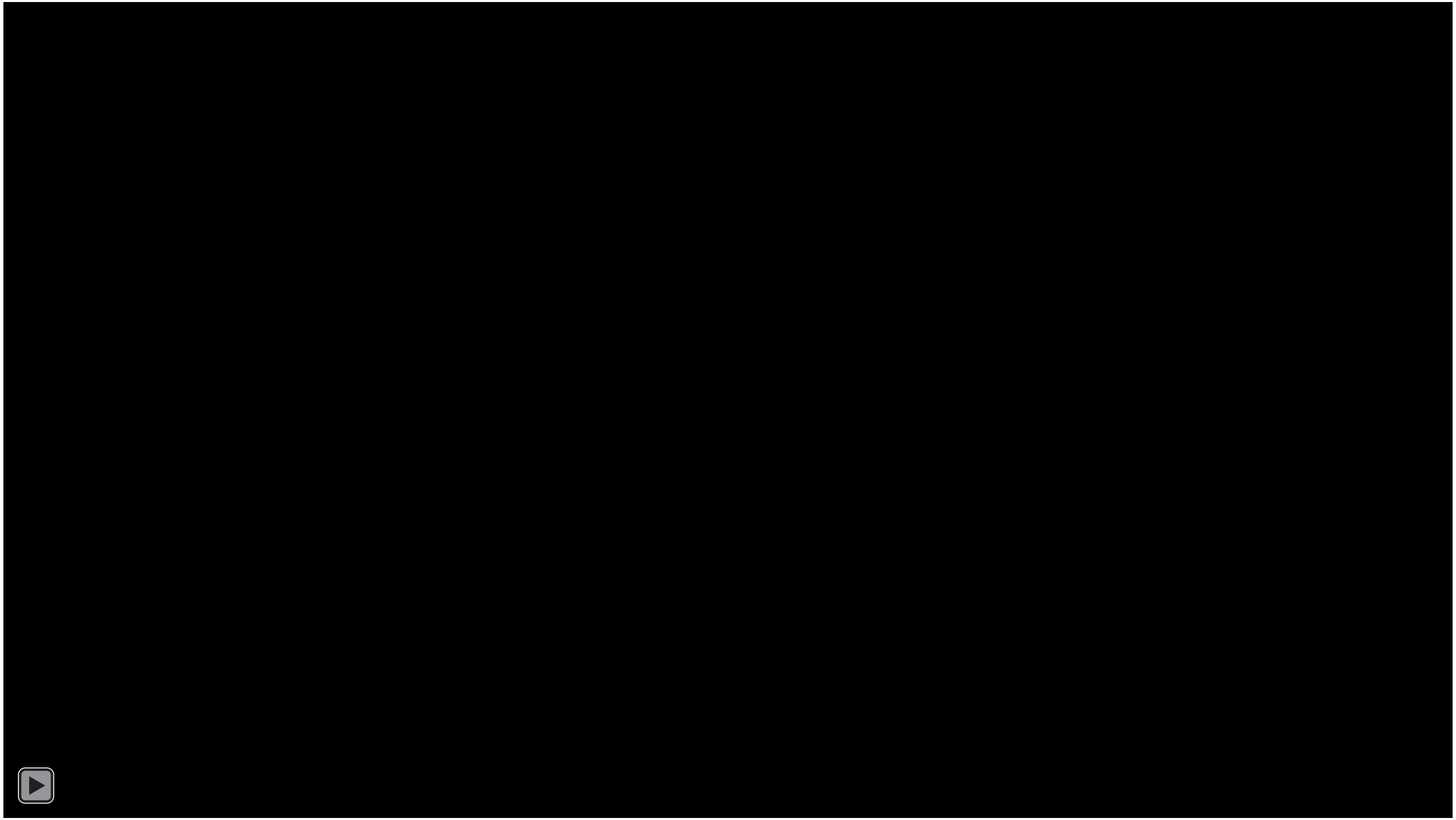
Test Matrix

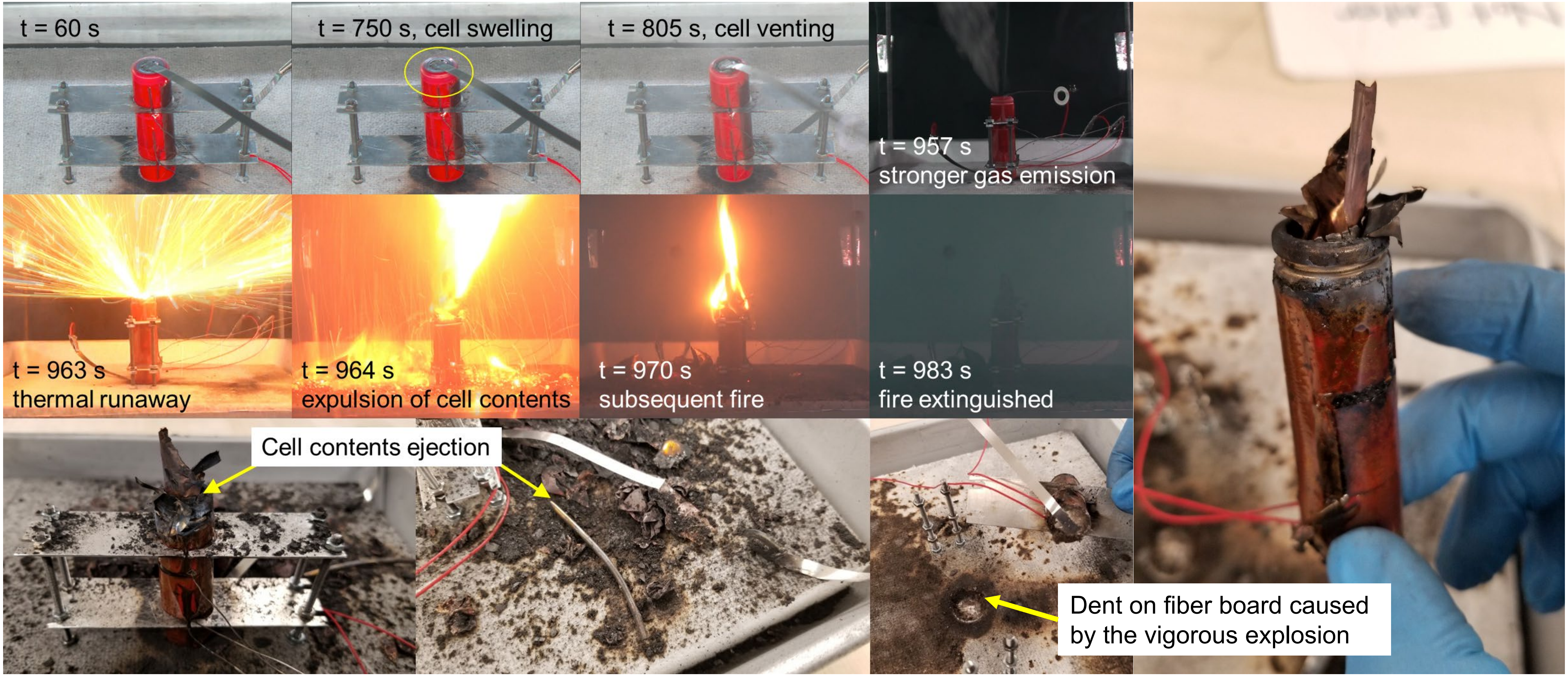
SOC (%)	Mass (g)	Internal Resistance (mΩ)	Capacity (Ah)	Final Voltage (V)
30%	45.23	57.30	2.43	3.70
30%	45.19	56.30	2.44	3.70
50%	45.27	58.70	2.42	3.77
50%	45.10	62.60	2.45	3.77
50%	45.20	54.80	2.45	3.77
50%	45.14	56.50	2.43	3.77
75%	45.21	61.10	2.40	3.93
75%	45.18	53.60	2.42	3.93
100%	45.14	57.30	2.45	4.19
100%	45.18	57.40	2.40	4.19
Avg	45.18	57.56	2.43	
Stdev	0.05	2.56	0.02	

Fire

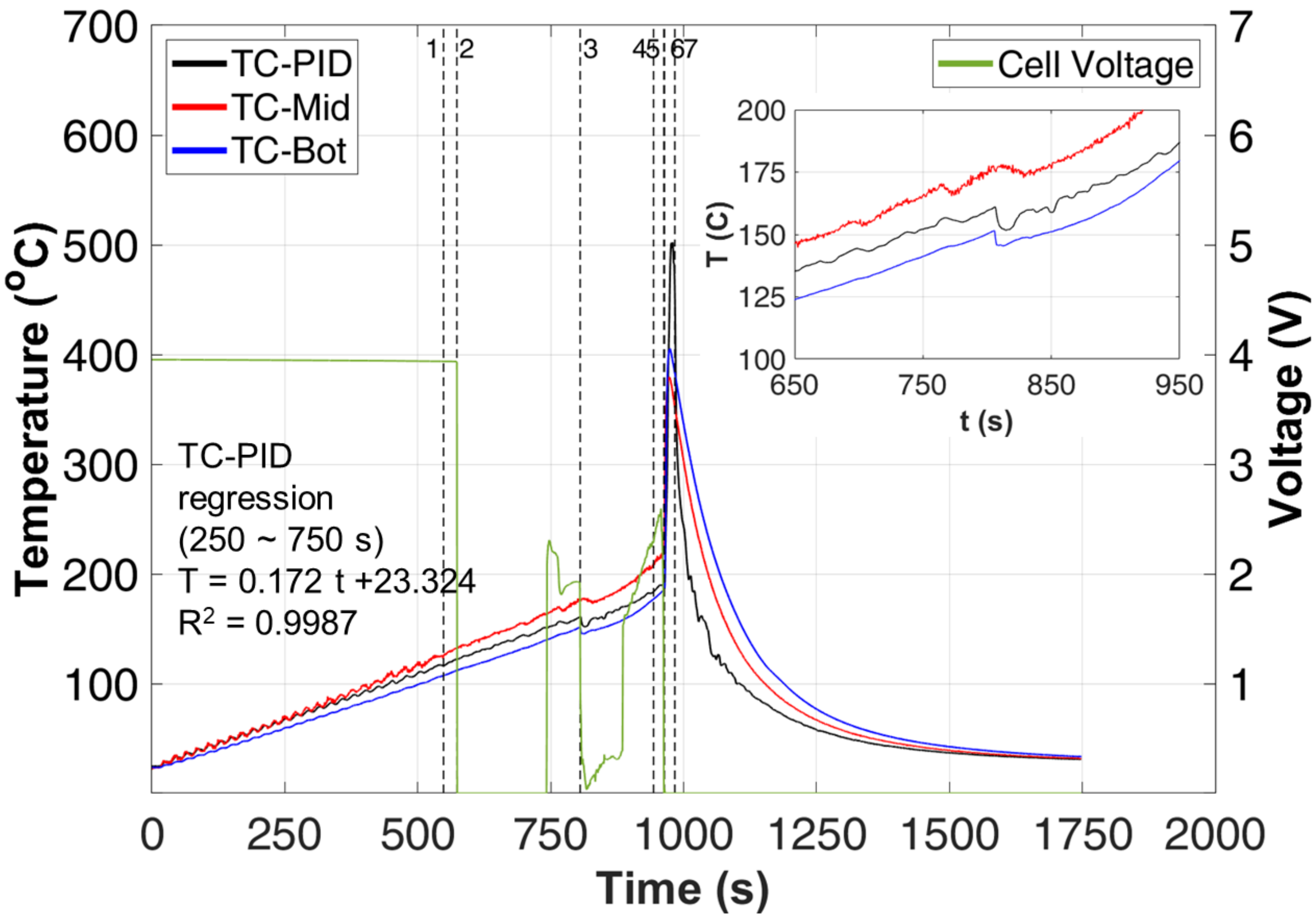
Example Result: Thermal Runaway at 75 % SOC



Example Result: Thermal Runaway at 75 % SOC



Example Result: Cell Temperature (75 % SOC)



1. Cell swelling (t = 548.5 s)
2. Cell V drop (t = 573.8 s)
3. Cell venting (t = 805.5 s)
4. Stronger gas emission (t = 943.6 s)
5. Thermal runaway, spark and fire (t = 963.0 s)
6. Expulsion of cell contents (t = 964.0 s)
7. Fire extinguished (t = 983.6 s)

- Tape heating rate is at ~ 0.172°C/s or **10.32 °C/min**.
- Cell voltage drops at ~ 120 °C.
- Prior to thermal runaway, mid TC has the highest reading and the bottom TC shows the lowest.
- TC readings show a momentary dip around the onset of venting.

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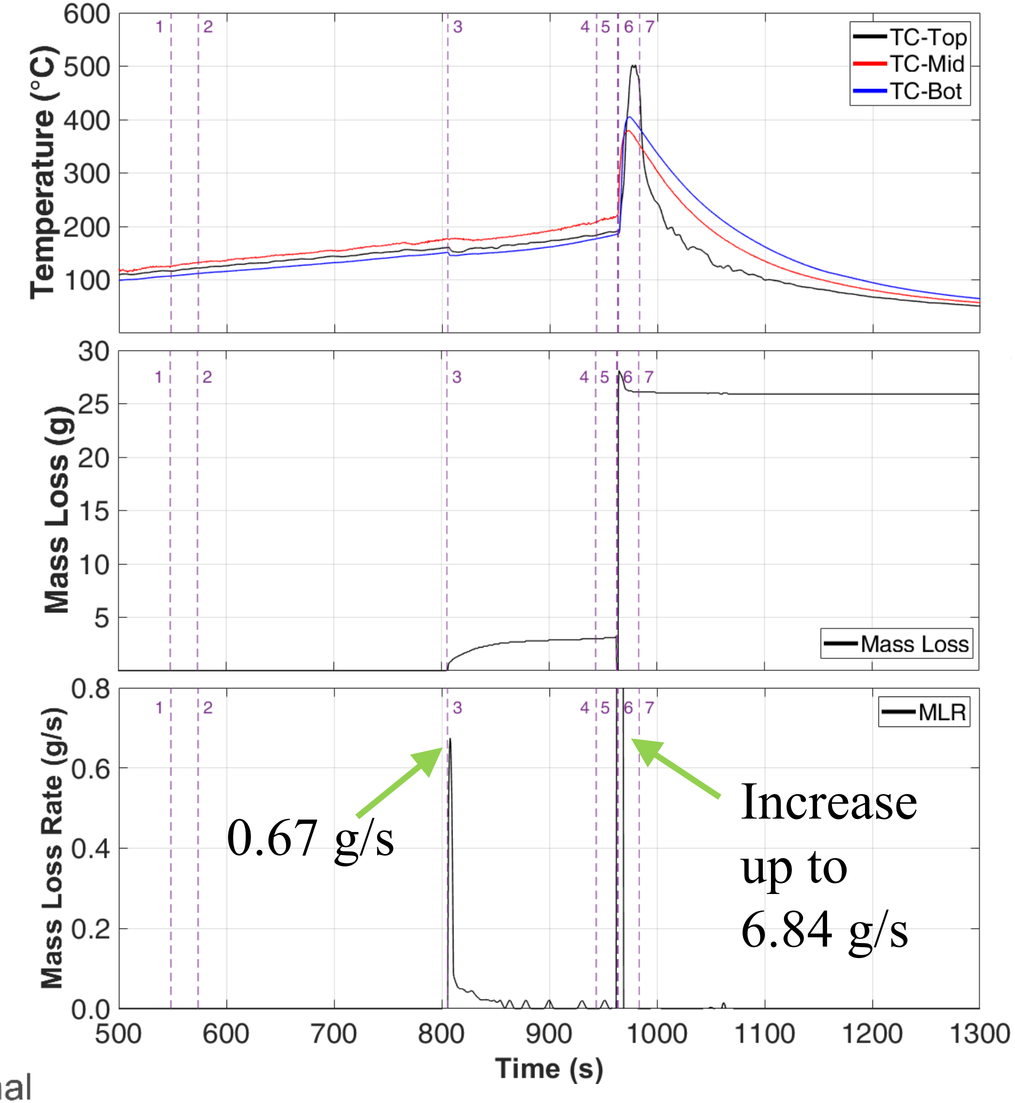
Example Result: Cell Mass Loss and Vent Gas Species (75 % SOC)



1. Cell swelling (t = 548.5 s)
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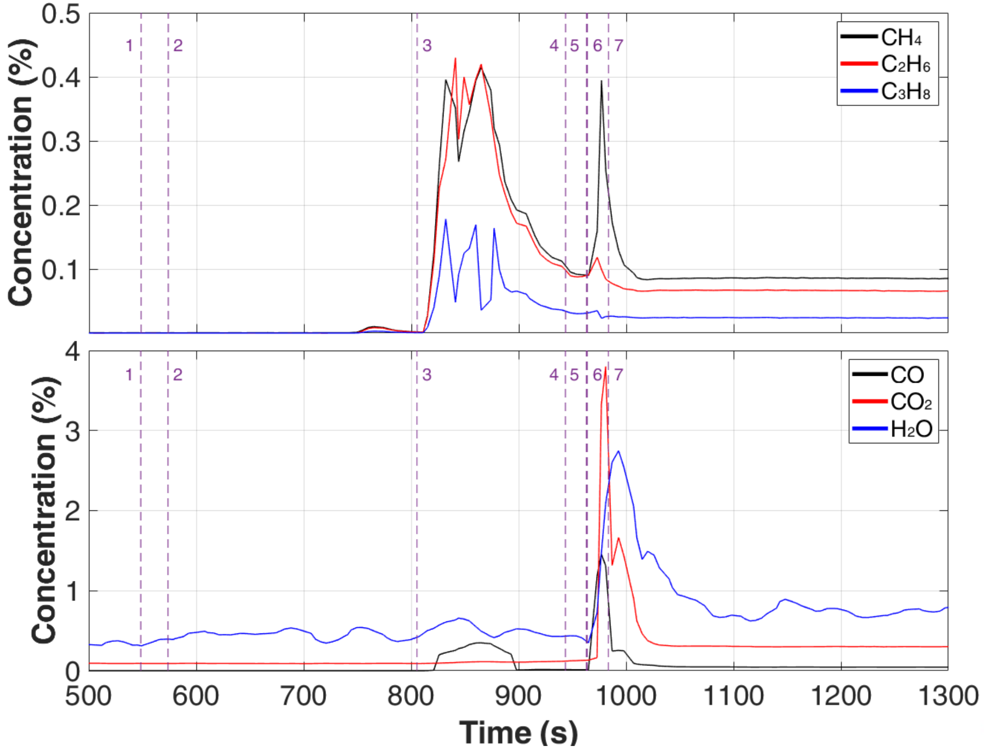
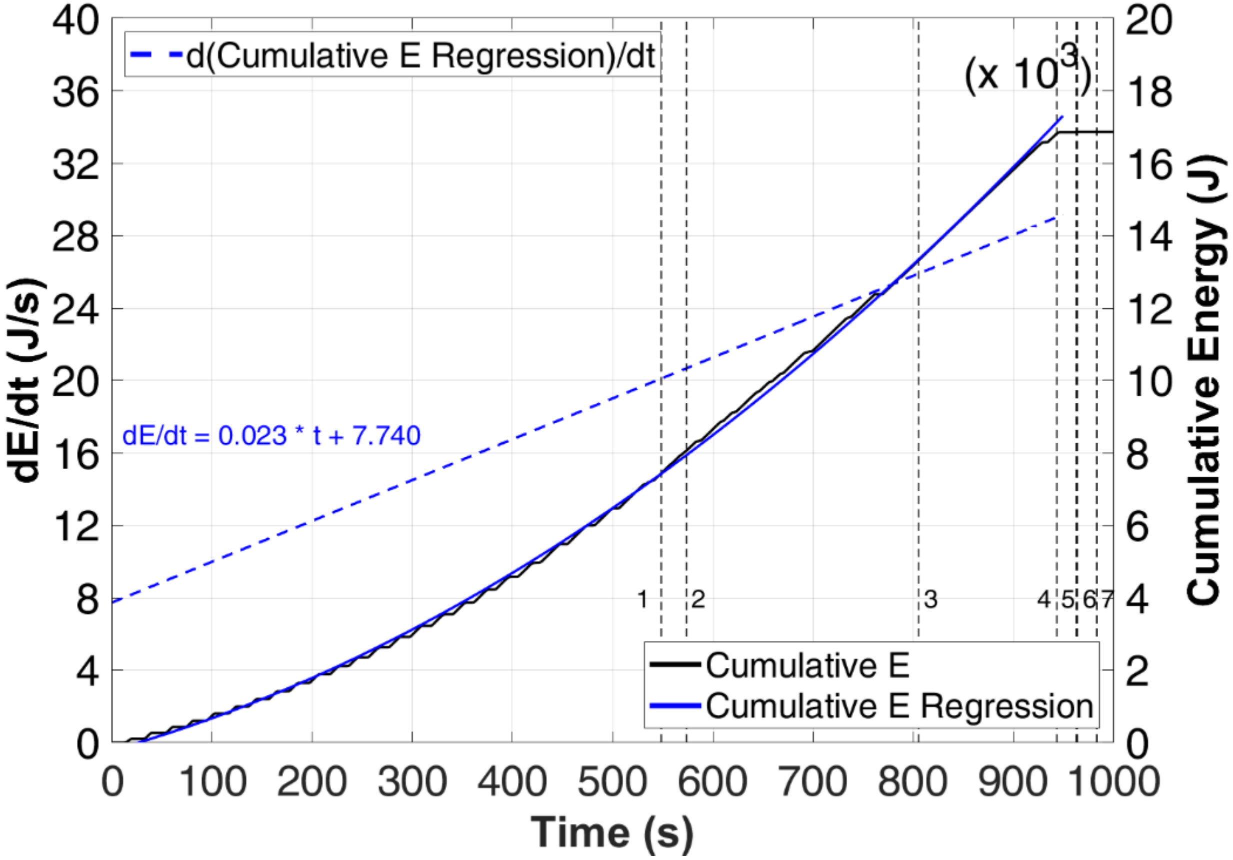


Power Input to the Heating Tape



1. Cell swelling
2. Cell V drop
3. Cell venting
4. Stronger gas emission
5. Thermal runaway and fire
6. Expulsion of cell contents
7. Fire extinguished

Cumulative Energy

$$E(t) = \int_0^t P\,dt = \int_0^t (V \times I)\,dt$$

Energy equation for a cell before thermal runaway

$$\rho c_v V \frac{dT}{dt} = \dot{q}_{tape} + \dot{q}_g - hA(T_s - T_\infty)$$

10 °C/min

Assume negligible before TR

$$\Longrightarrow \quad \dot{q}_{Tape} = \frac{dE}{dt} = \underbrace{mc_v \frac{dT}{dt}}_{\text{Assume constant}} + \underbrace{hA(T_s - T_\infty)}_{\text{Increases linearly w.r.t. time.}}$$

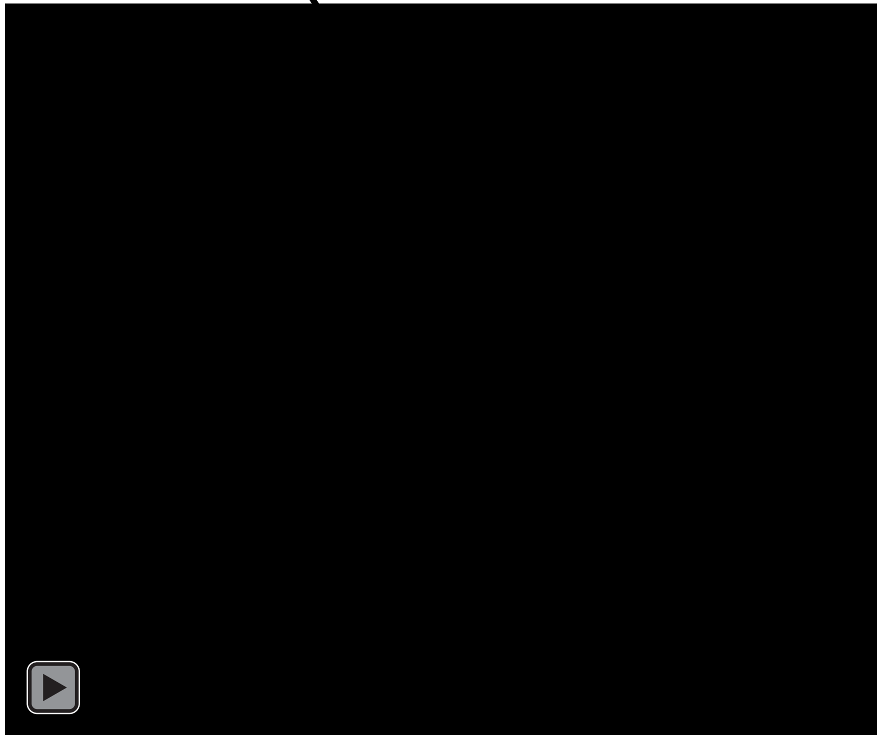
Results: Venting and Thermal Runaway at All SOCs

SOC: 30 % 50 % 75 % 100 %

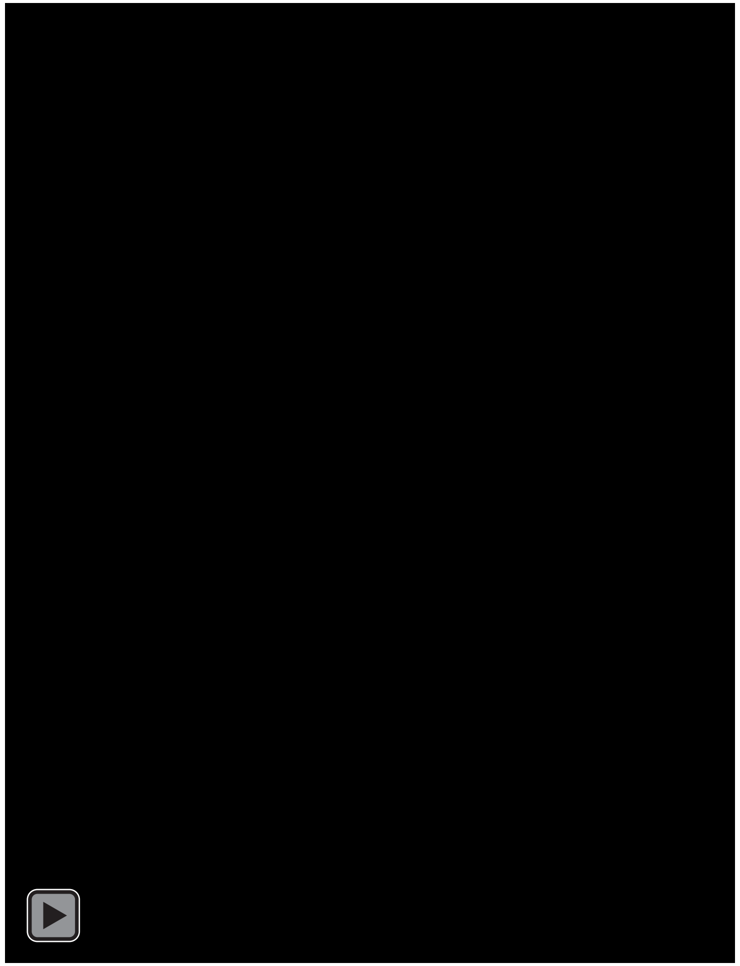
The videos are played at <u>3 times rate.</u>

Results: Venting and Thermal Runaway

At venting, bubbles of boiling electrolyte were observed.



SOC 100%_CT7



SOC 30%_CT6

SOC 75%_CT8

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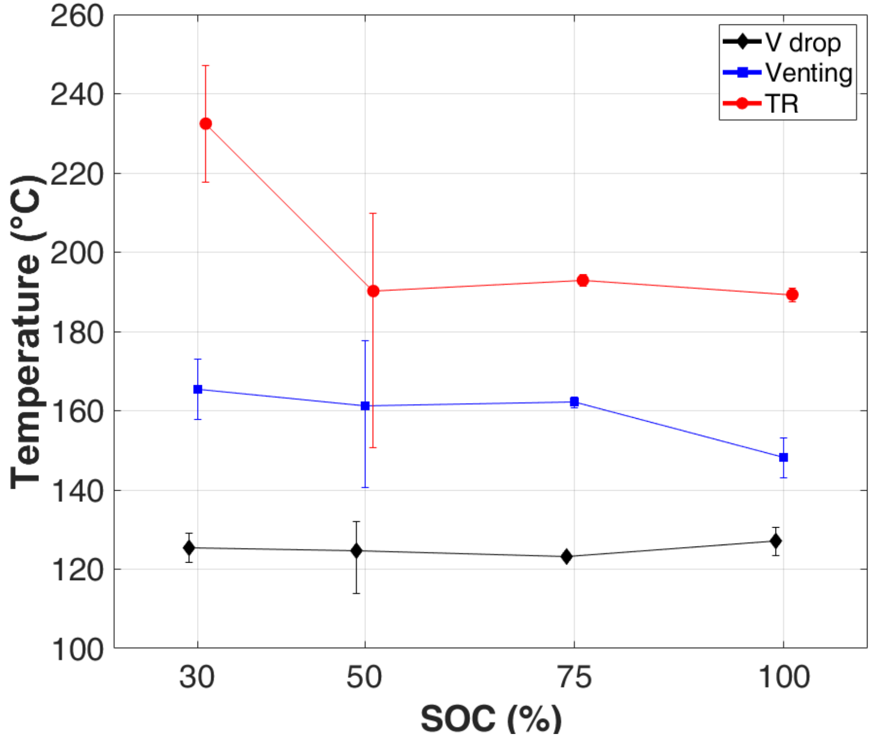
Temperatures at Key Events

	Cell V drop		Cell venting		Thermal runaway		Burning
SOC (%)	time (s)	T (°C)	time (s)	T (°C)	time (s)	T (°C)	time (s)
30	575.2	121.6	789.7	157.8	998.0	217.7	
30	605.8	129.0	862.3	173.1	1110.0	247.2	
50	576.7	121.4	757.7	152.7	950.3	192.0	
50	631.7	132	891.6	177.6	1072	209.9	
50	627.8	131.4	870	174.2	1047	208.3	
50	528.8	113.9	698.1	140.5	855.7	150.6	23.4
75	573.8	122.1	805.5	160.8	963.0	191.5	20.6
75	577.2	124.2	814.1	163.4	982.3	194.3	37.7
100	627.0	130.6	757.0	153.2	968.0	191.0	19.0
100	568.9	123.5	683.2	143.0	923.1	187.6	45.8



- Voltage drop temperatures are insensitive to SOC.
- Venting and thermal runaway occurred at a lower temperature at a higher SOC.

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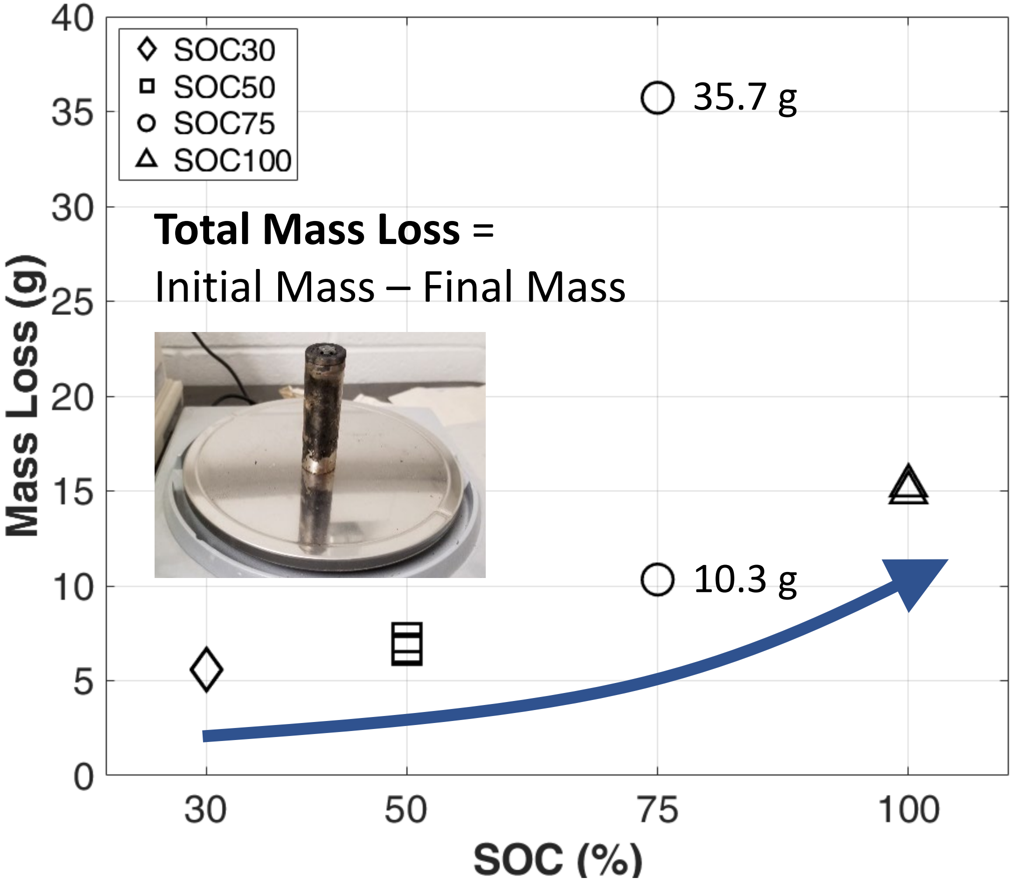
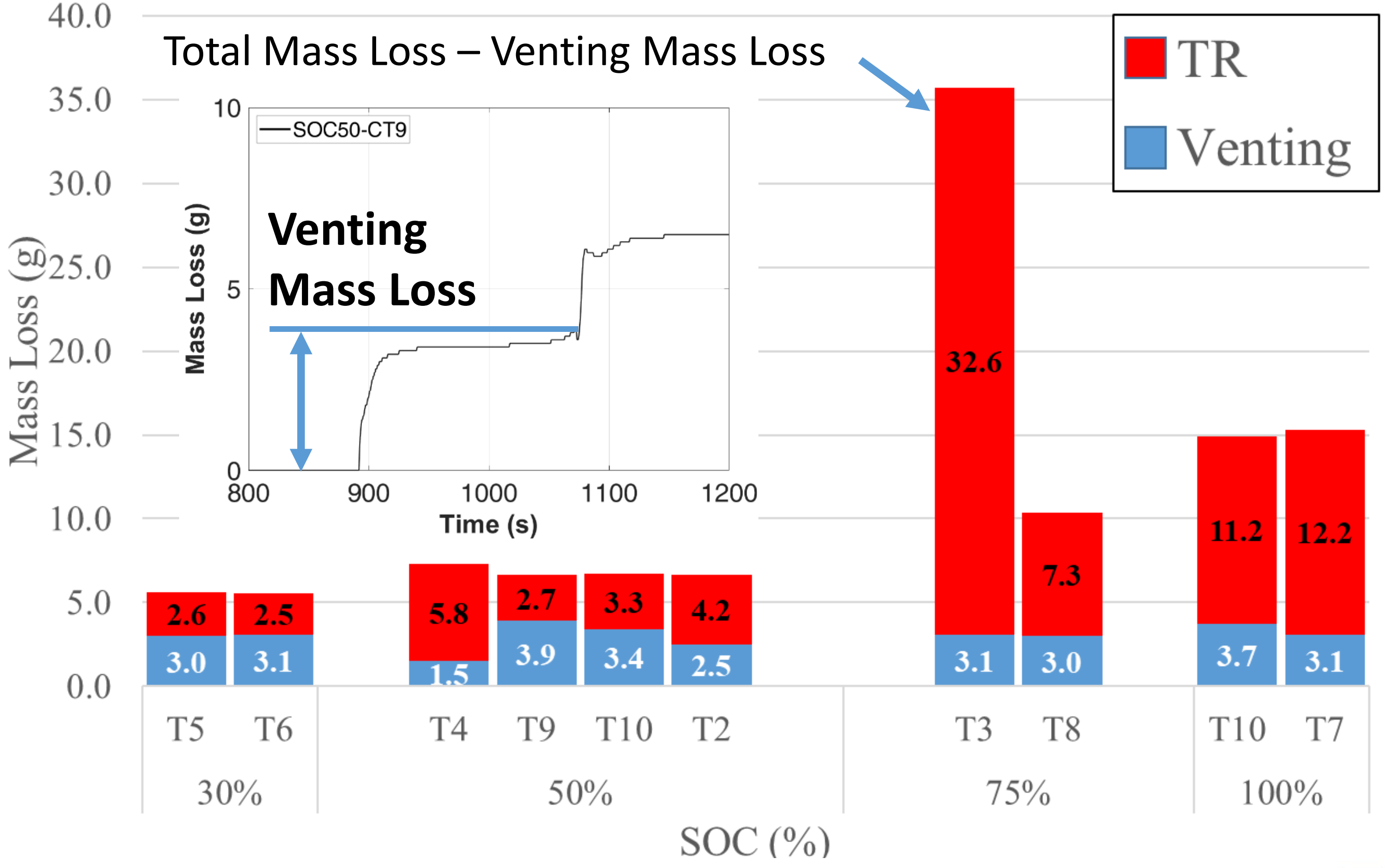
Cell Mass Loss at Different SOC





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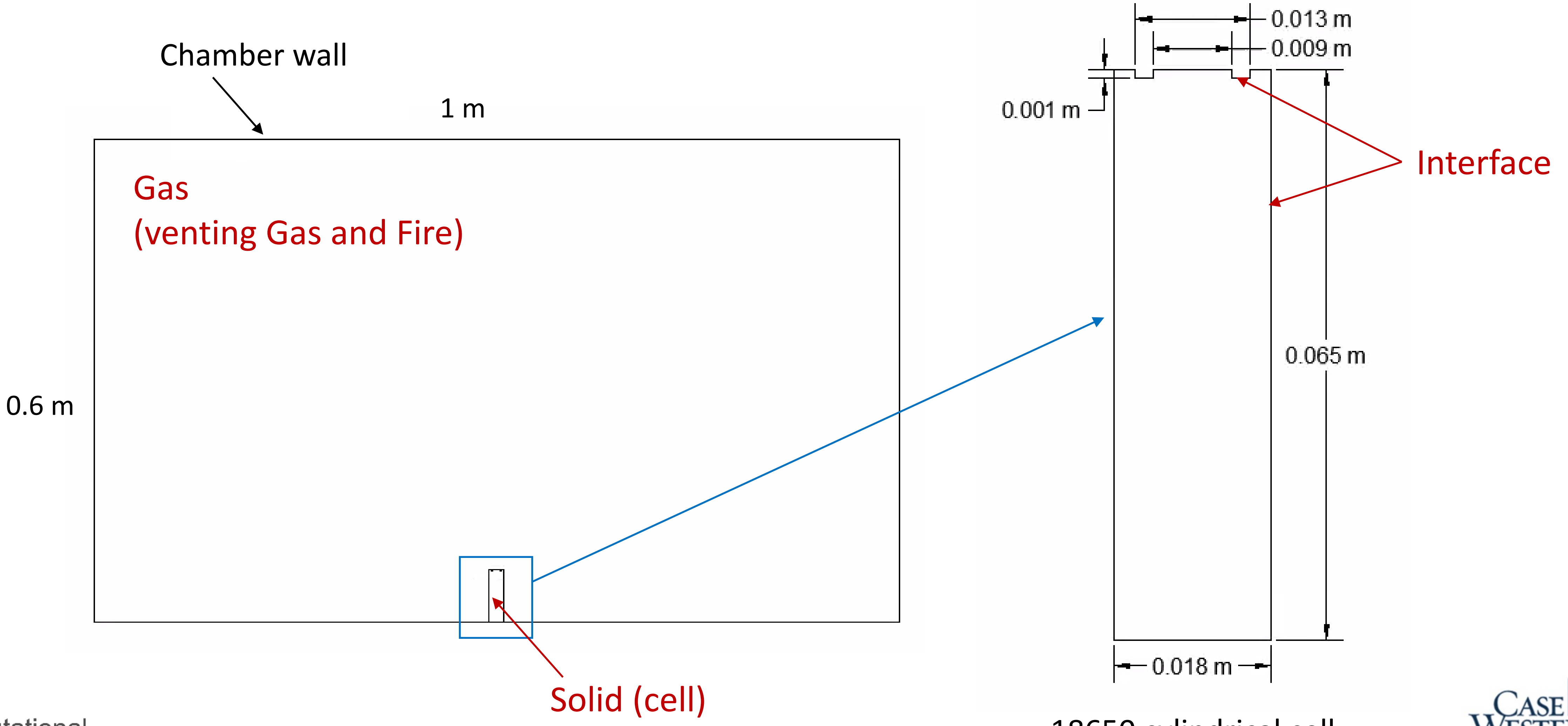
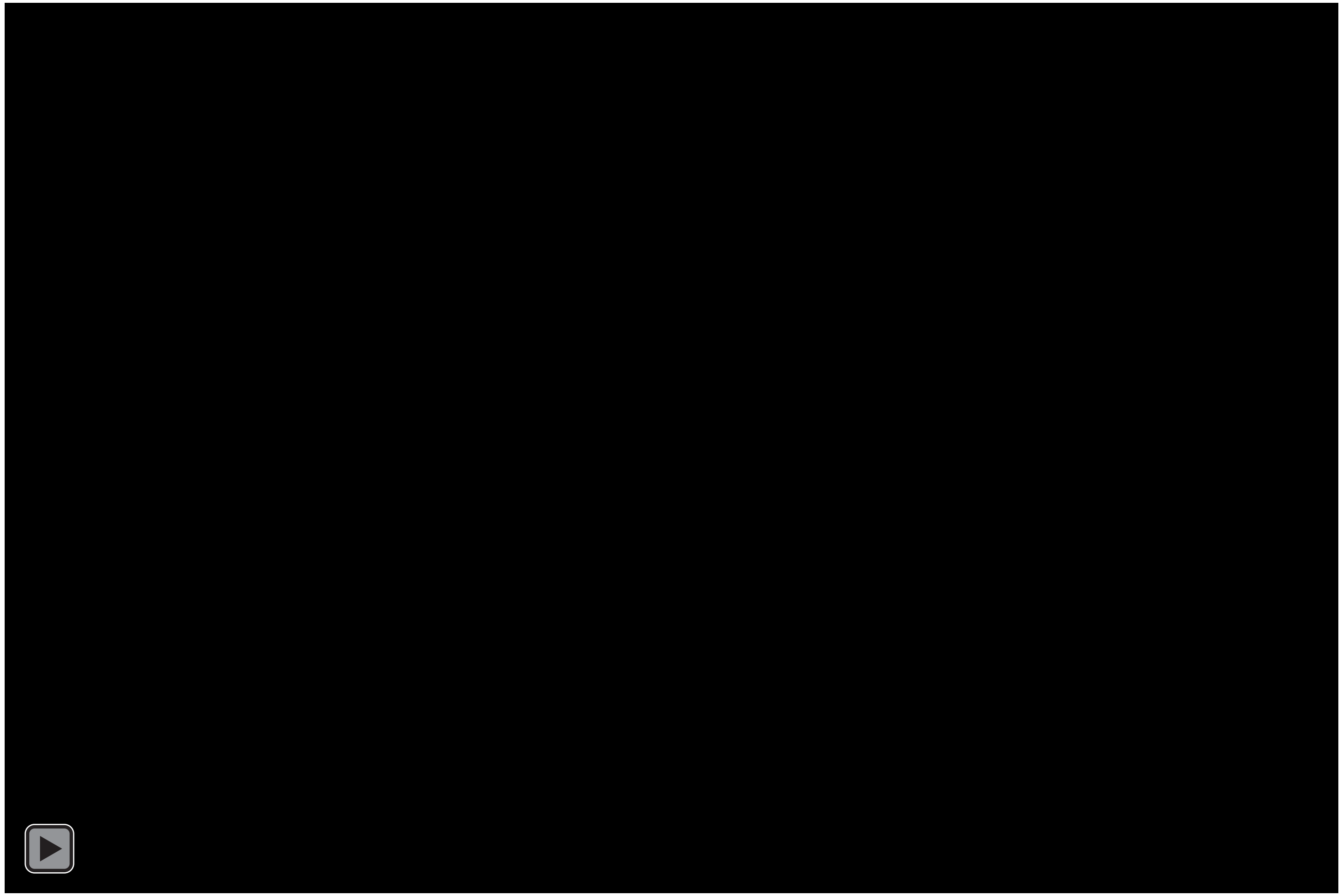
Numerical Model (Work-in-Progress): Gas + Solid + Interface



18650 cylindrical cell

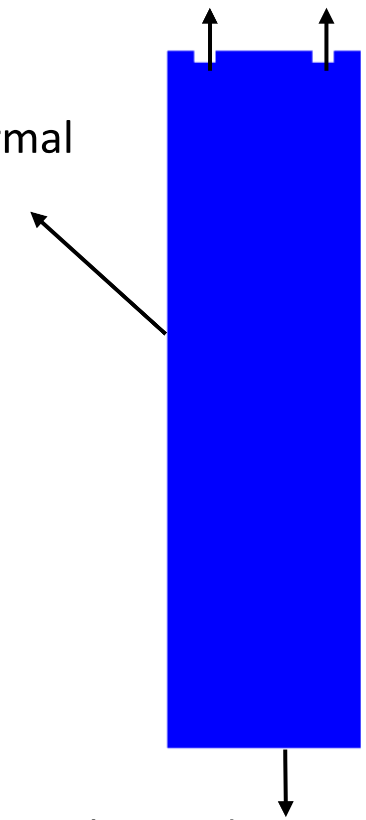
Numerical Model (Work in Progress): Gas



*This preliminary simulation used mass flow inlet with 0.02kg/s of pure CH_4.

- Reynolds-Averaged Navier-Stokes (RANS) equations with k-epsilon turbulence model.
- Non-premixed species combustion model.
- SIMPLE scheme with second order discretization method.
- Transient solver.

Numerical Model (Work in Progress): Solid



$$T = 300K + 10\left(\frac{K}{min}\right) \times t$$

- Transient solid conduction equation.
- Cell pseudo-properties deduced from the experimental data.

$$\dot{q}_{Tape} = mc_p\frac{dT}{dt} + hA(T_s - T_\infty)$$

$$m = 0.045\ kg; \dot{q}_0 = 7.74\frac{J}{s}; \frac{dT}{dt} = 0.172\frac{K}{s}$$

$$\rightarrow c_p = \mathbf{1,000}\,\frac{\boldsymbol{J}}{\boldsymbol{kg\cdot K}}; \rho = \frac{0.045\ kg}{1.654\times10^{-5}m^3} = \mathbf{2,720.60}\,\frac{\boldsymbol{kg}}{\boldsymbol{m^3}}$$

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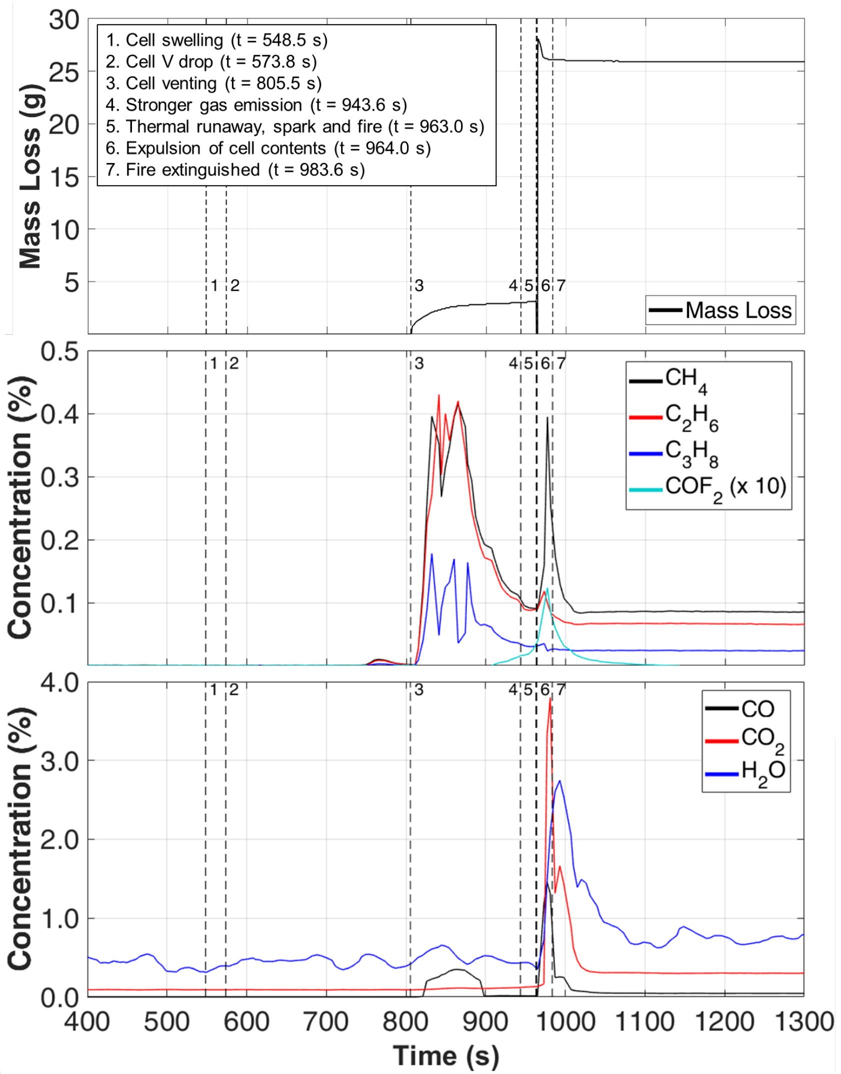
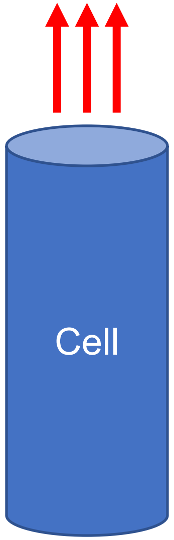
Numerical Model (Work in Progress): Interface



$\frac{dm}{dt}$ (g/s)



- UDF boundary conditions at the cell-gas interface:

$$\frac{dm}{dt} = \boxed{f_1(T_{cell}, SOC)}$$
$$F_i = \boxed{f_2(T_{cell}, SOC)}$$

To be deduced from the experimental data.

- F_i : mass fraction of species *i* in the venting gas
  T_{cell}: cell temperature, solved by the solid model.
- f_1 and f_1 can be expressed explicitly using functions (e.g., Arrhenius equations), through look-up tables, or through ML.

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Summary

- Experiments are performed to study Lithium-ion battery (LIB) thermal runaway and its subsequent fires, using a 600L environmental chamber.
- A standard operating procedure (SOP) along with a chamber clean-up procedure are developed for the experiments.
- Temperature, voltage, and ***mass loss of the battery cell***, ***concentrations of the venting gas species***, and the ***energy input to the battery cell*** are measured in-situ. Results of cells at different State of Charge (SOC) are compared.
- The time-resolved experimental data is processed to deduce parameters for model development. These include ***pseudo-properties of the battery cell***, ***venting gas compositions, and venting mass rate as functions of the cell temperature and the cell SOC***.
- The fire events in the experiments and the modeling results will be compared in both ***single and multiple cell*** levels. After the model is comprehensively validated, it will be used to study fire ***propagation*** between cells, and to understand the ***scalability*** of battery fire.