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Evolution of the flammability environment surrounding lithium-ion battery failures

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Abstract

Failure of lithium-ion batteries can result in venting of gases which pose a significant flammability risk [1]. To accurately assess this risk, 18650 format batteries will be thermally abused to cause venting failures, during which the vented material will be collected using a grab sampling system. The vented material will be analyzed after the collection to determine gaseous species present. A reduced order model will be paired with the experimental data to analyze the flammability environment around the cells.

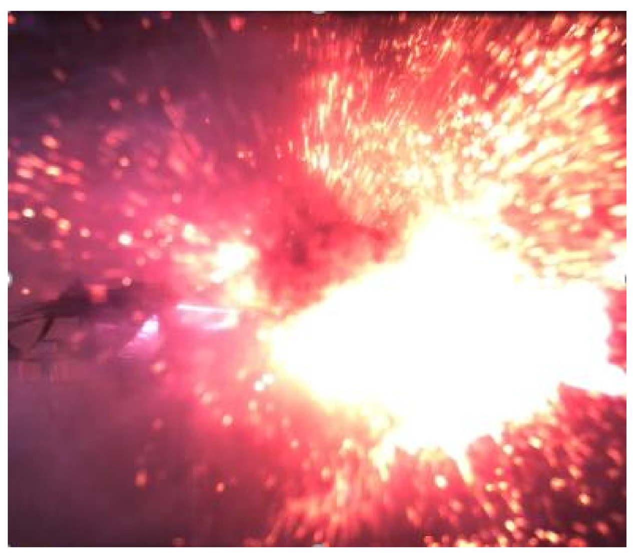

Figure 1: Failing 18650 format cell

Reduced-Order Model

The theoretical assessment of flammability environments is conducted using a reduced order mathematical model developed for this research. This model was built using MATLAB and simulates the flow out of failing cells into a specified environment (Figure 2). The mass ratio (ϕ) of flammable gas to air is compared to the flammability limits of the vented species to characterize the temporally evolving flammability environment. The outputs for the model include: the time at which the defined system becomes flammable (if this occurs), the time at which the system surpasses the upper flammability limit and is no longer flammable (if this occurs), plots showing mass ratio ϕ as a function of time, and flammability curves showing lower and upper flammability limits as a function of time and gas species (Figure 3).

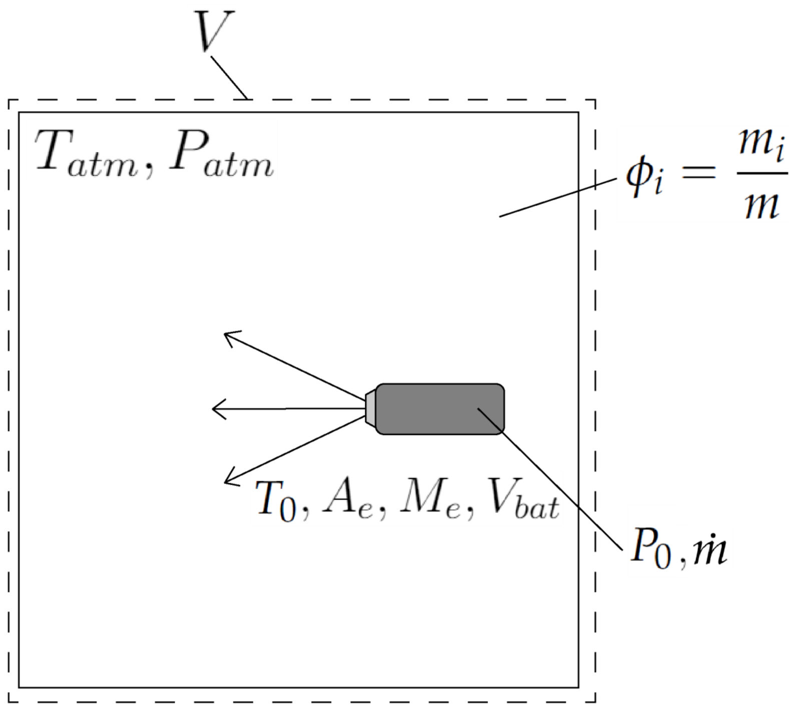

Figure 2: Schematic for model

The mass flow out of the failing cell is calculated using an equation derived by Mier [2], and is based on internal battery properties, and exit geometry:

$$\dot{m} = C_d \frac{P_0}{\sqrt{RT_0}} A_e \sqrt{\gamma} M_e \left(1 + \frac{\gamma - 1}{2} M_e^2\right)^{\frac{\gamma+1}{2-2\gamma}}$$

Preliminary testing was run with the model to guide a test setup for the experimental testing. Once cell venting hydrogen was simulated for a range of system volumes. It was determined that for this scenario, any volume above 0.0562 m³ does not become flammable. This set a minimum volume for the testing enclosure, which was finally chosen to be 0.2227 m³.

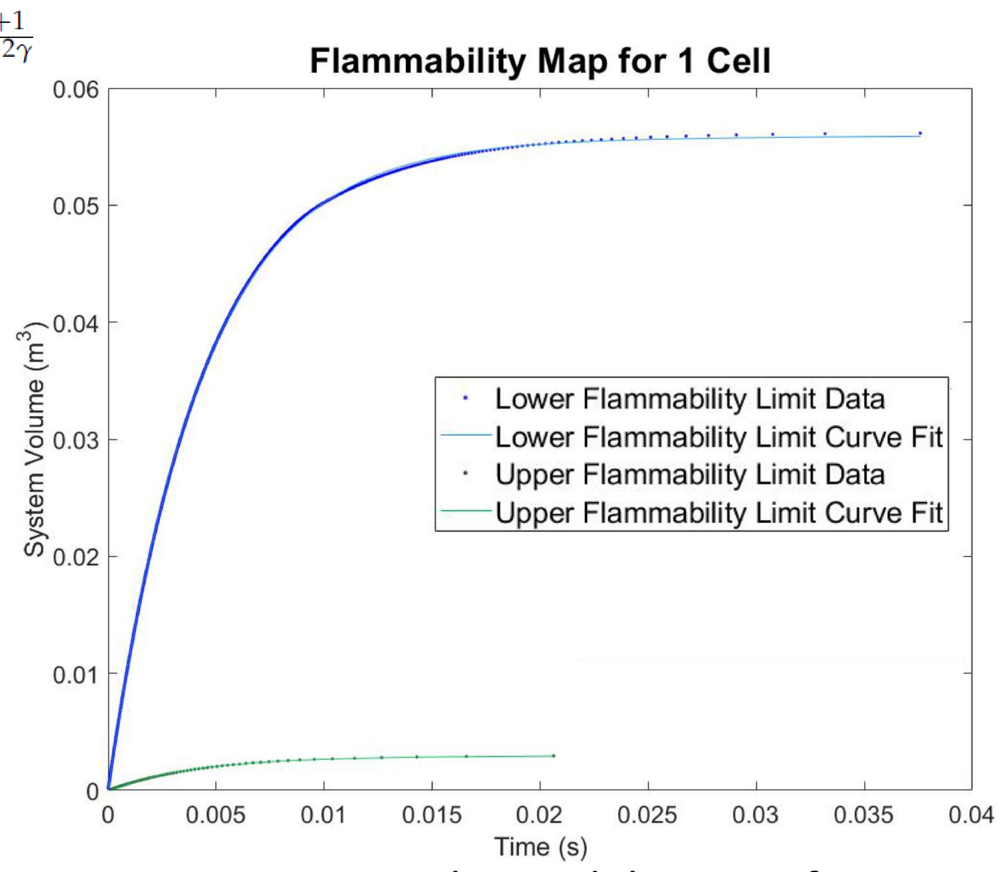

Figure 3: Flammability map for 1 cell venting hydrogen

Dynamic grab sampling device

An experimental testbed was developed to capture and analyze the gases vented from failing batteries. To accurately analyze the electrolyte, samples were captured during abuse testing using grab samplers developed for this research. The grab sampler is made up of a series of parts (Figure 4) including: a ball valve (A), a sample cylinder (B), connectors (C and D), a pressure transmitter (E), a check valve (F), and a pneumatic valve (G). The grab samplers are opened using electric solenoid valves. Preliminary tests were conducted to refine timing within testing process. For these tests, all parts for the sampler were used whereas for the final test series, the connectors and pressure transmitter (C, D, and E) were not used.

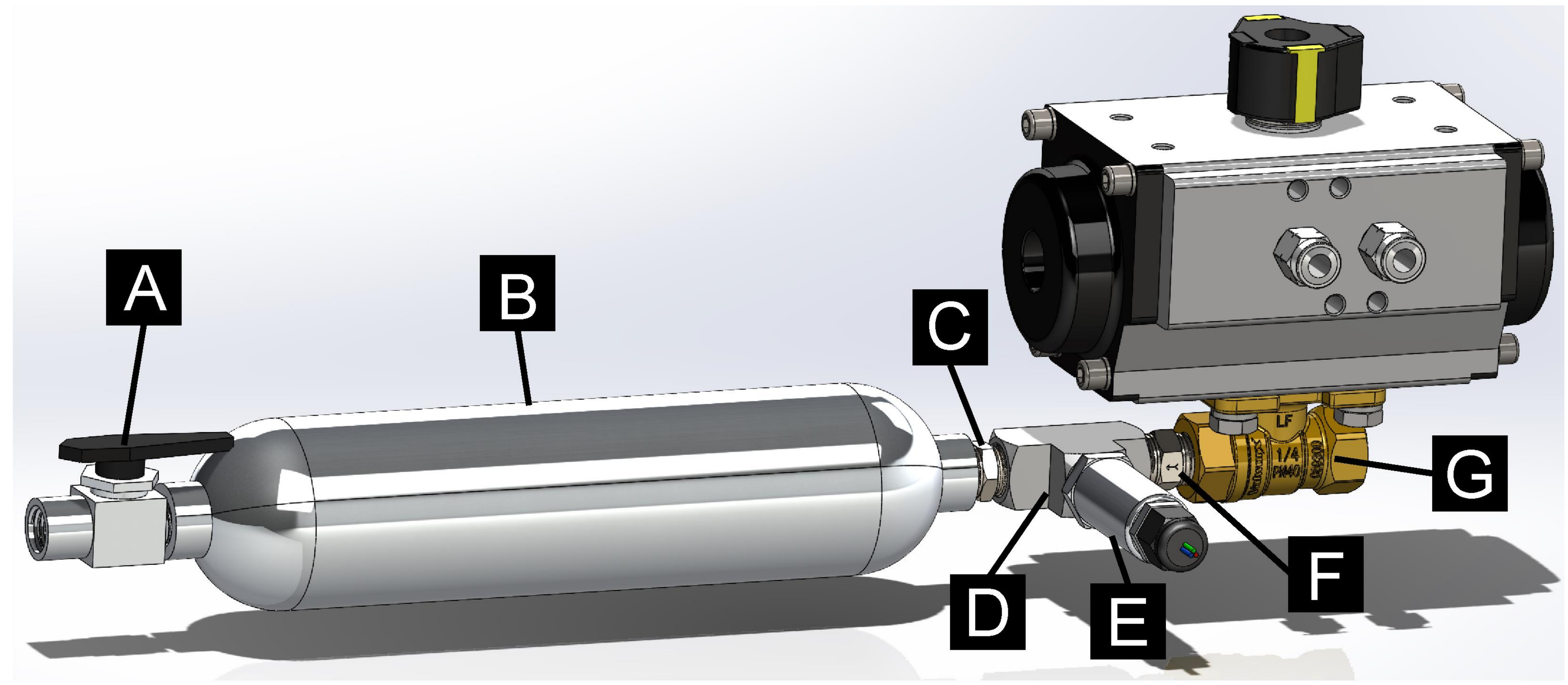

Figure 4: Model of extended grab sampler

Experimental Testing

Experiments are performed in a large open volume where a battery cell is heated to failure and the grab samplers collect vapor when the cell fails. An aluminum block was machined to house cartridge heaters, thermocouples, and a cell that is used to heat the cell until failure. Temperature in the block is monitored through the thermocouples. Once the cell begins venting, the system is triggered either acoustically or manually, and the solenoid valves are powered on which opens the pneumatic valves and allows flow into the sample cylinders. The system then closes after a set time, sealing the samples. The samplers were placed at two locations: one at approximately 4 cm from the cell and one at about 14 cm. National Instruments Modules paired with a LabVIEW VI are utilized to control all electronics in the testing apparatus and to read data from the sensors.

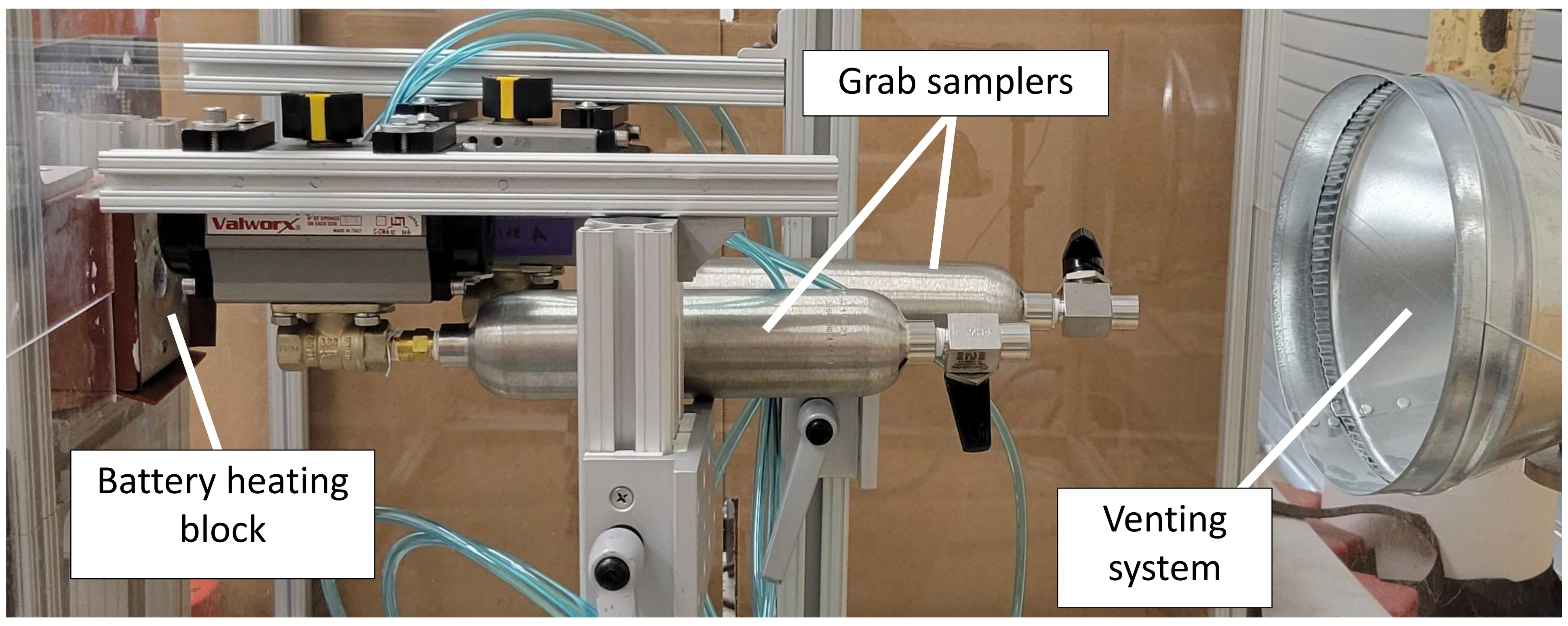

Figure 5: Testing setup with samplers and battery mounting block

The composition of sample electrolyte was analyzed using Fourier-Transform Infrared Spectroscopy (FTIR) and Mass Spectrometry (MS).

Results and Discussion

The MS data shows that chemicals with different molecular weights were captured within the grab sampler. Partial pressures for the determined masses were found for each sample, then means and confidence intervals were determined. The mean partial pressures and their confidence intervals were plotted (Figure 6).

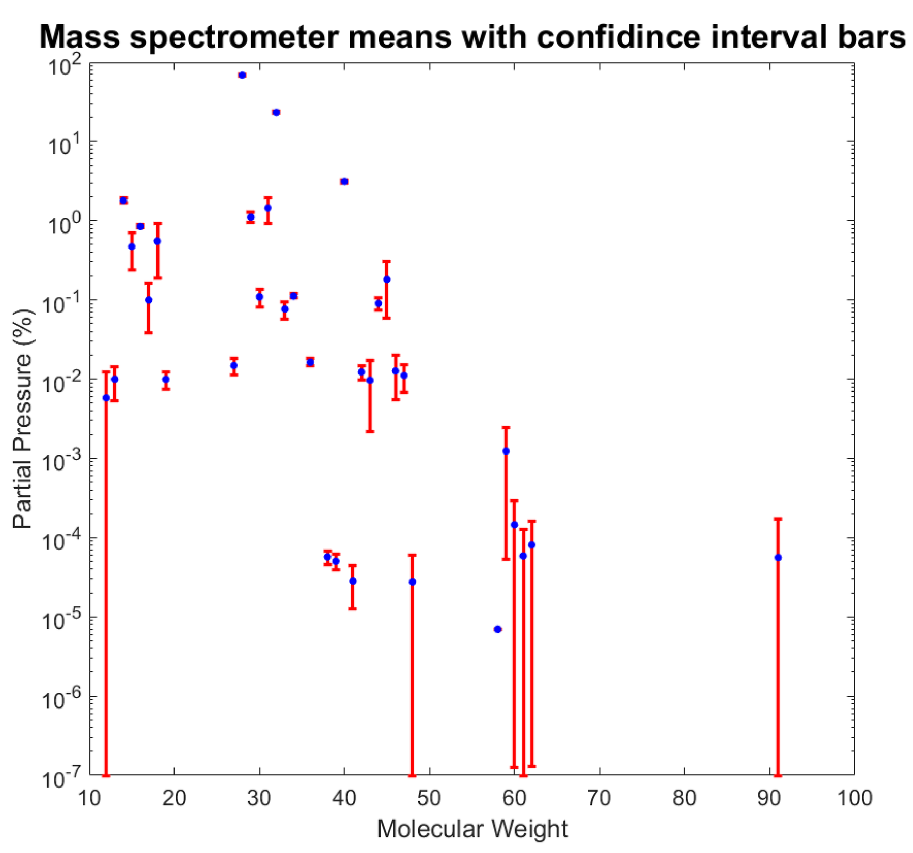

Figure 6: Partial pressures for masses found from MS analysis

The FTIR data is a spectrum of absorbance versus wavelength. The FTIR spectra are plotted on one graph to see differences in peak locations and relative absorbance between spectra across samples.

The MS data of masses coupled with the location of peaks in the FTIR spectra provides an overview of the composition of the electrolyte mixture. The main components of air were detected in this analysis: nitrogen (the primary species in all samples), oxygen, water, argon, etc. A few of the species that have been defined as most likely possibilities besides normal air components include: ethane, methylamine, and propene.

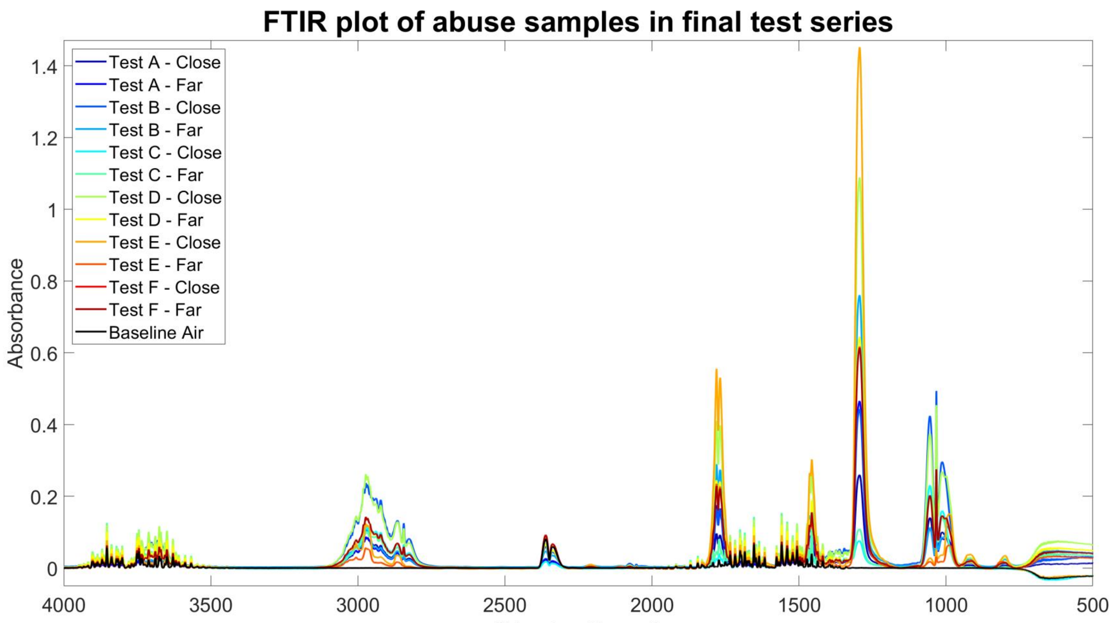

Figure 7: FTIR Spectra for all electrolyte samples

Future Work

Once the vented gas composition, in terms of species present and relative concentrations, is determined, the results will be used as inputs for the model to more accurately simulate the flammability environment surrounding the failing cells. Tests will be run with the model with the composition for a range of system volumes and number of cells to give a better understanding of safety limits of different scenarios. The confidence intervals found for the partial pressures will also be used as upper and lower bounds for composition inputs to the model to account for error in the experimental measurements.

References and Acknowledgements

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[1] Q. Wang, B. Mao, S. I. Stoliarov, J. Sun. *A review of lithium ion battery failure mechanics and fire prevention strategies,* Progress in Energy and Combustion Science, Volume 73, 2019, Pages 95-131.

[2] F. A. Mier, 2020. *Fluid Dynamics of Lithium Ion Battery Venting Failures*. [Doctoral dissertation]. New Mexico Institute of Mining and Technology.

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