Evolution of the flammability environment surrounding lithium-ion battery failures

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Introduction

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 were thermally abused to cause venting failures. During the venting, material was collected using a grab sampling system. The vented material was analyzed after the collection to determine chemical species present. A reduced order model was developed and paired with the experimental data to assess the flammable environment around the cells.

Figure 1: Failing 18650 format cell

Reduced-Order Model

The theoretical assessment of flammability environments were conducted using a reduced order mathematical model developed for this research. This model was built using MATLAB and models 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 species present to characterize the temporally evolving environment. The outputs for the model included: the time when 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). 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:

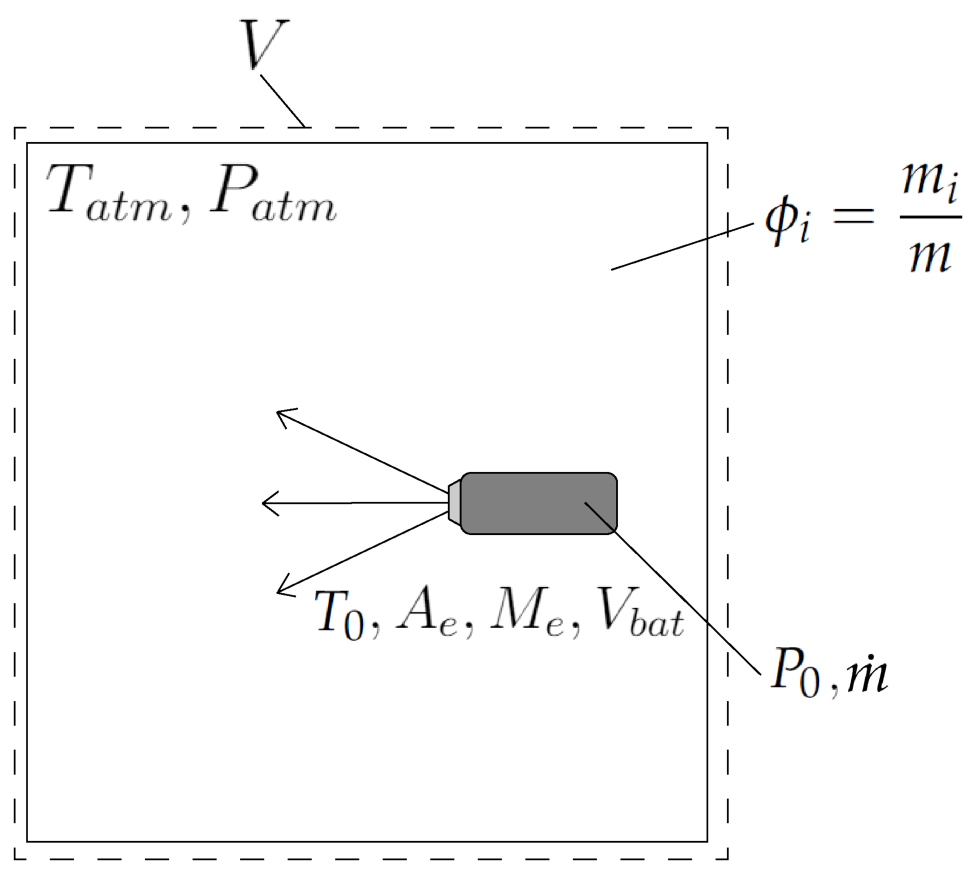

Figure 2: Schematic for model

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

Preliminary testing was run with the model to guide the setup for the experimental testing. One cell venting hydrogen was simulated for a range of system volumes. It was determined that for this scenario, any volume above 0.0413 m³ does not become flammable. This set a minimum volume for the testing enclosure, which was finally chosen to be 0.2227 m³. Additional cases were tested as reported in [3].

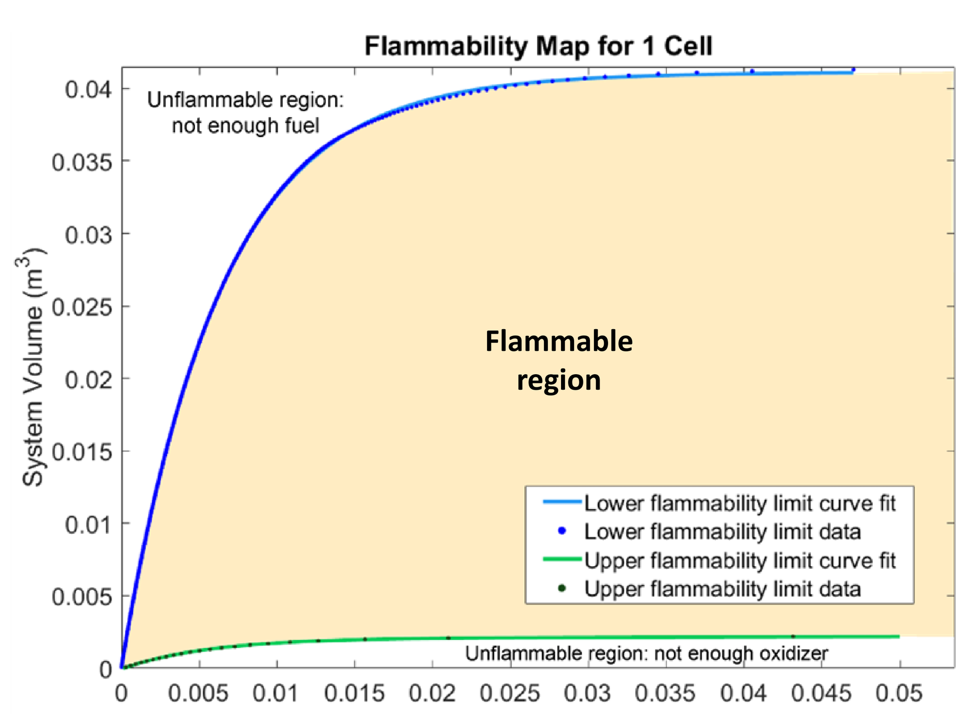

Figure 3: Flammability map for 1 cell venting hydrogen

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 (Part A), a sample cylinder (Part B), connectors (Parts C and D), a pressure transmitter (Part E), a check valve (Part F), and a pneumatic valve (Part 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 (Parts C, D, and E) were not used.

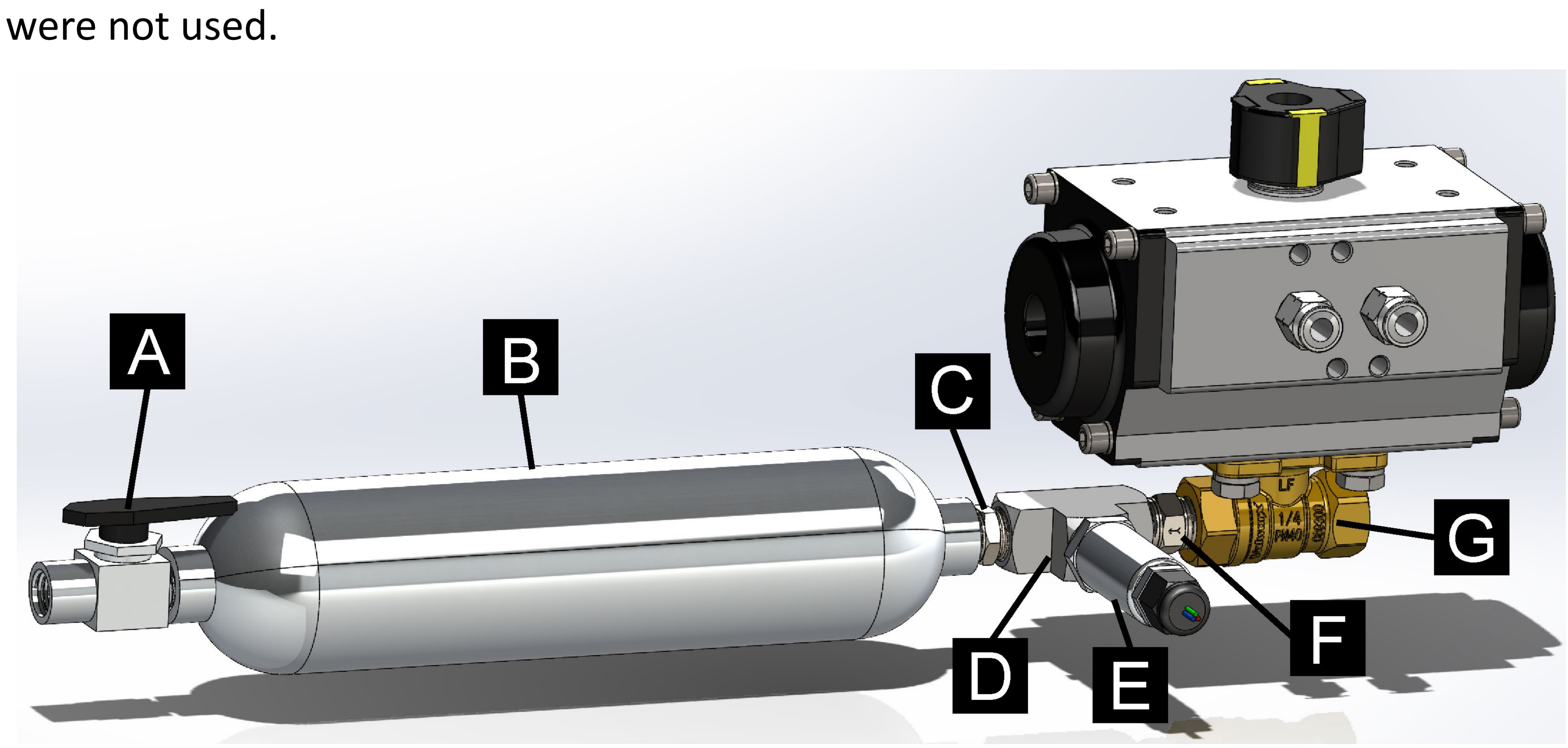

Figure 4: Model of extended grab sampler

Experimental Testing

Experiments were performed in a large open volume where a battery cell was heated to failure and the grab samplers collected vapor when the cell failed. An aluminum block was machined to house cartridge heaters, thermocouples, and the 18650 cell. Temperature in the block was monitored through the thermocouples. Once the cell began venting, the system was triggered either acoustically or manually, and the solenoid valves were powered on which opened the pneumatic valves and allowed flow into the sample cylinders. The system then closed 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 were utilized to control all electronics in the testing apparatus and to read data from the sensors.

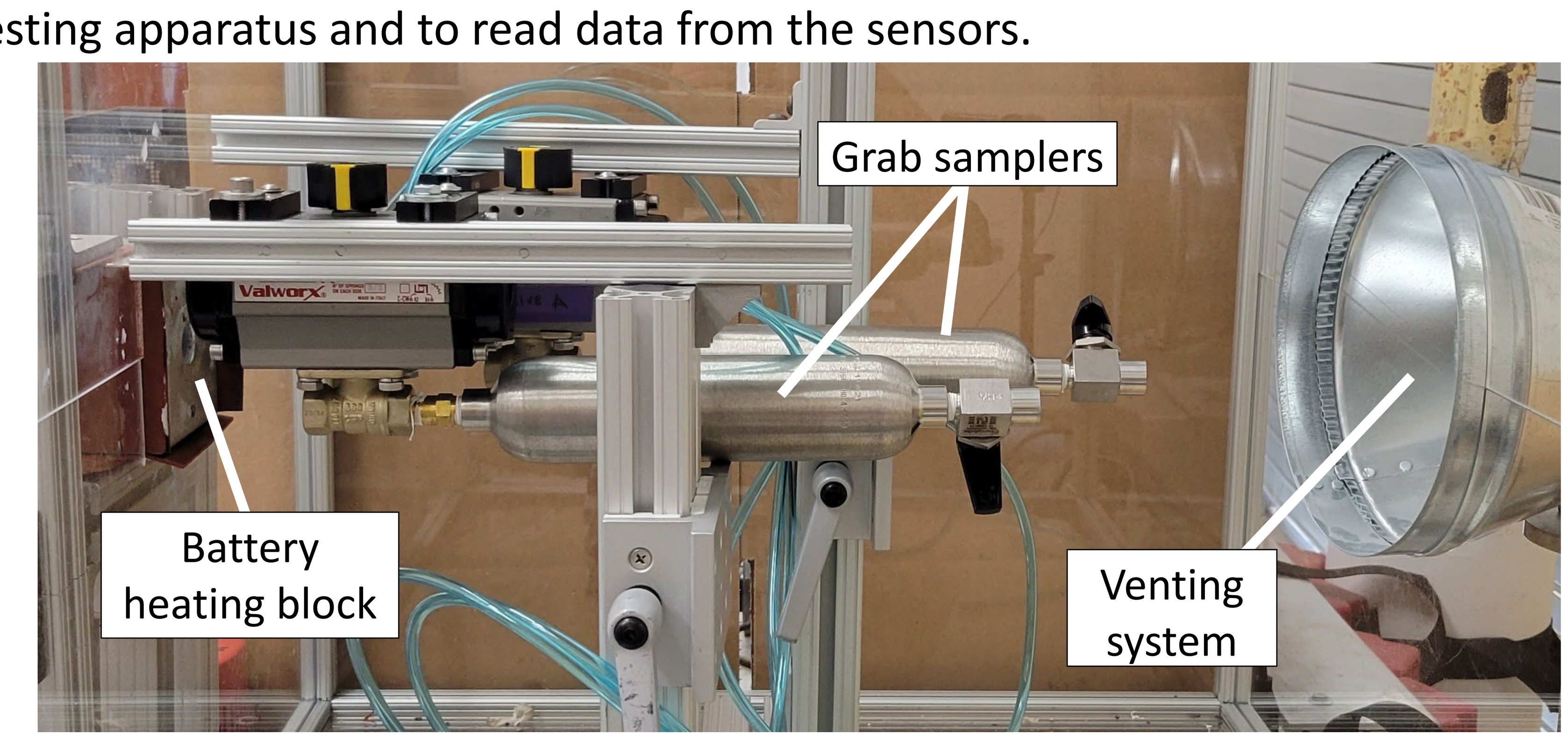

Figure 5: Testing setup with samplers and battery mounting block

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

Results and Discussion

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

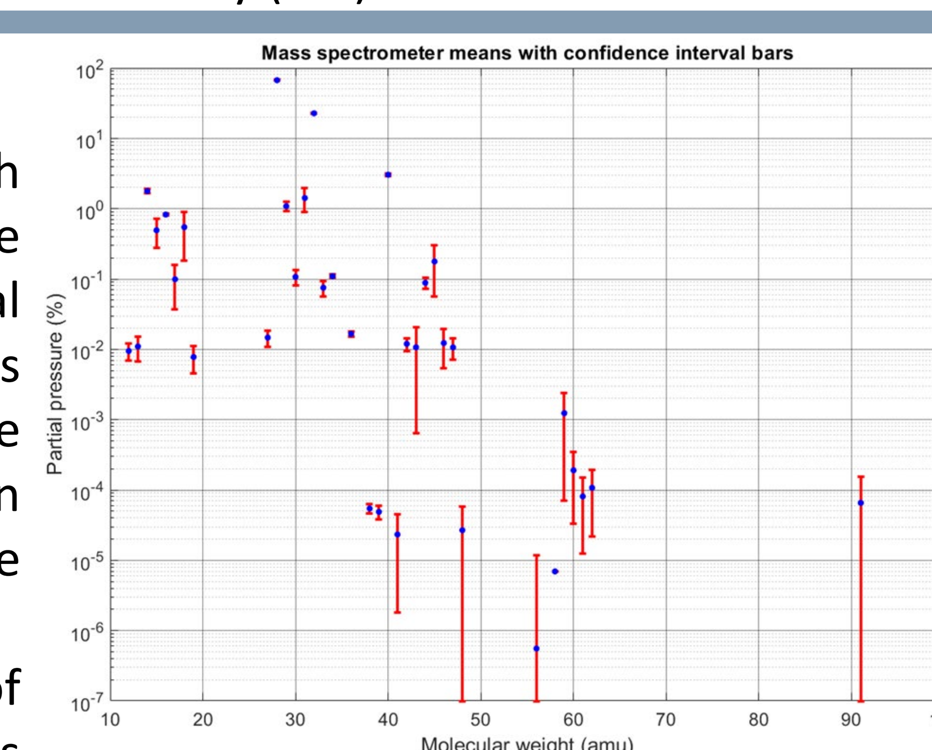

Figure 6: MS data for an electrolyte sample

The FTIR data is a spectrum of absorbance versus wavelength. This coupled with the MS data allows calculation of the composition of the vented gas materials. The main components of air are all detected here and make up most of the mass peaks, including nitrogen (the primary species in all samples), oxygen, water, and argon.

A database was built with the spectra of all possible species based on the MS analysis and spectra for possible electrolyte solvents. Using the eFTIR software, the experimentally collected spectra was analyzed relative to the database to determine the mixture composition. The analysis showed that the species with this highest correlation to the collected spectra was dimethyl carbonate (DMC). The flammability environment based on the DMC partial pressure was modeled for a cell and is shown in Figure 7.

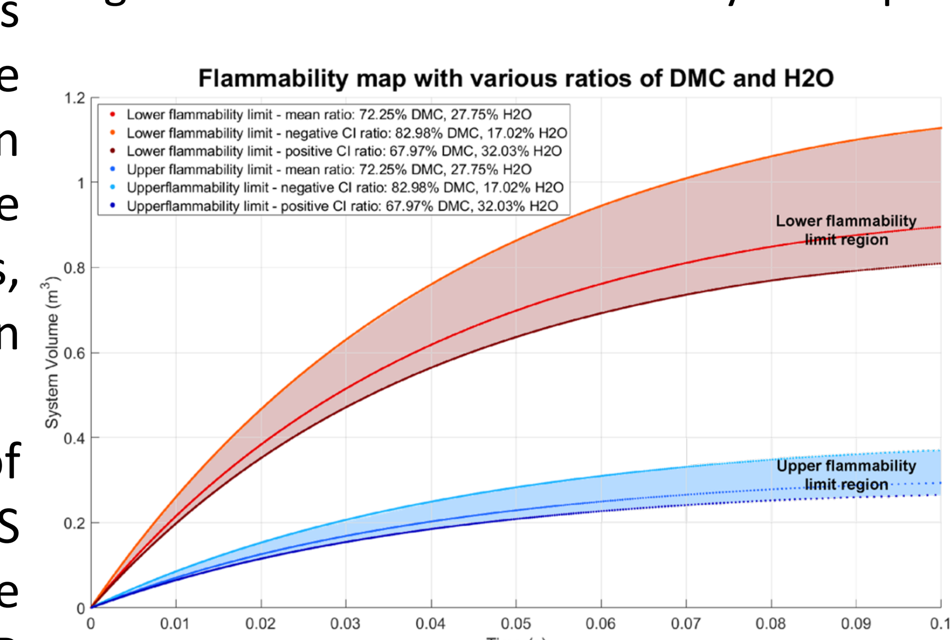

Figure 7: Flammability map for a single cell

Future Work

Future chemical analysis work should investigate the use of Raman spectroscopy or nuclear magnetic resonance (NMR) spectroscopy to provide a more comprehensive understanding of the chemical composition of the vented gases. A Thermo-gravimetric Analysis (TGA) on the baseline electrolyte material would be useful to produce data for the breakdown of the material as a function of temperature.

The next phase of this research will be investigating the heat transfer load caused by the venting electrolyte spray during failures.

References and Acknowledgements

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