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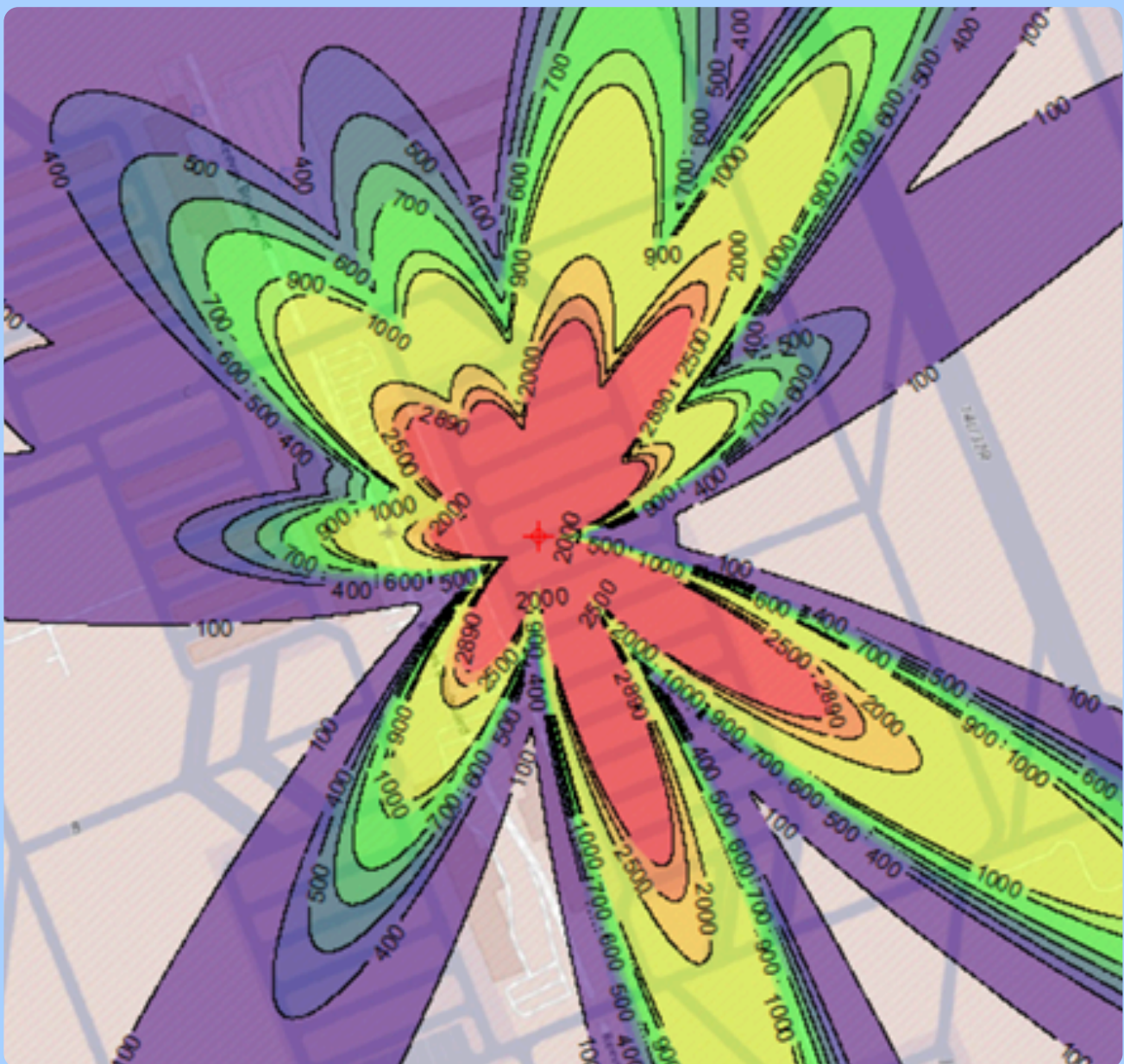
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Environmental and Health Impacts of Thermal Runaway Events in Outdoor Lithium-Ion Battery Energy Storage System Installations



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Environmental and Health Impacts of Thermal Runaway Events in Outdoor Lithium-Ion Battery Energy Storage System Installations

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Executive Summary

This research presents a methodology to assess the health and environmental impacts from thermal runaway events in outdoor, large-scale, Li-ion BESS units. Through application of the methodology, a relationship between exposure limit distance and wind speed, ambient temperature, event duration, cell chemistry, and toxic gas species can be established. This study did not consider other health factors, such as thermal exposure. The methodology involves a literature review to aggregate data, plume dispersion modeling, and a risk analysis of the model results.

Data on thermal runaway characteristics of Li-ion batteries, including propagation rates, gas emission composition and yields, heat release rate, mass loss rate, total heat released, total gas produced, and cell gas venting temperatures was collected from peer reviewed studies and historical Li-ion BESS incidents. Representative BESS unit characteristics were gathered from UL 9540A test documentation. Additionally, information on fire and plume dispersion models was collected to determine suitable modeling programs. Fire Dynamics Simulator (FDS) was selected for analysis of near-field (up to 200 m) health impacts and AERMOD was selected for analysis of far-field (up to 2.5 km) health and environmental impacts.

The modeled scenario involved a generic 3.101 MWh outdoor BESS unit undergoing thermal runaway in a rural area with flat terrain and low-lying vegetation. It was assumed that there were no surrounding buildings or complex terrain. Non-flaming and flaming thermal runaway scenarios were modeled with both LFP and NMC cell chemistry. No fire suppression was modeled. A bounding analysis on wind and temperature was conducted to determine the impact of meteorological conditions on plume dispersion in FDS. For AERMOD, an identical reference set of meteorological conditions was used to run all simulations; therefore, the impact of varying meteorological conditions was not assessed, only the cell chemistry and thermal runaway conditions.

For the non-flaming scenarios, it was assumed that thermal runaway propagated throughout one bay but that heat transfer was not sufficient to cause propagation across barriers separating the bays. The rate of gas released was calculated based on an estimated total gas volume production and incident duration. An average, steady state gas volume release was modeled for each scenario and gas production rates for specific species were determined based on percentage gas composition data obtained from the literature review. For the flaming scenarios, it was assumed, based on historical incidents, that thermal runaway propagated throughout the full BESS unit. Data from the literature review was used to estimate heat release rate and heat of combustion values, and subsequently mass loss rate values. An average, steady state mass loss rate was modeled for each scenario and gas production rates were determined based on yield data obtained from the literature review. Incident durations for the non-flaming and flaming simulations were based on typical cell vent times, large-scale testing data, and historical incidents.

The FDS and AERMOD models were used to predict concentrations of gases at a breathing height of 1.5 m. The AERMOD model also predicted metal particulate deposition onto ground level surfaces such as soil and water. Human health impact was evaluated by measuring the distance at which occupational or community exposure limits for gases were exceeded, i.e., IDLH and PAC, respectively. Environmental impact was evaluated by determining the relevant LC₅₀ and EC₅₀ values based on the location, as well as the reference depth for soil and water. Deposition at a point of interest was calculated to provide an example of the environmental impact methodology.

In the non-flaming scenarios, AERMOD model results tended to produce shorter community exposure limit distances than FDS, while in the flaming scenarios, FDS tended to produce shorter community exposure limit distances. While AERMOD may be capable of high-level predictions of long-range plume dispersion and grounding, FDS is likely more suitable for near-field analysis (up to 200 m) in scenarios involving combustion (and buoyancy driven flow). Conversely, atmospheric models that account for turbulence in the atmosphere (but not in the plume), such as AERMOD, in conjunction with real-world meteorological data, are likely better suited for plumes produced from non-flaming thermal runaway conditions, especially in the far-field.

The study findings related to exposure distances are specific to the modeled hazard scenarios and associated inputs; the relevant stakeholder or user should not apply the findings from this research in a site-specific hazard analysis without verifying that the modeled scenarios (and associated inputs) are applicable.

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List of Abbreviations

ACGIH: American Conference of Governmental Industrial Hygienist

ABS: acrylonitrile butadiene styrene

AEGL: Acute Exposure Guideline Levels

Ah: ampere-hour

AIHA: American Industrial Hygiene Association

ANSI: American National Standard Institute

ARC: accelerating rate calorimeter

AQI: Air Quality Index

BESS: battery energy storage system

BEV: battery electric vehicle

CATL: Contemporary Amperex Technology Co., Limited

CFD: computational fluid dynamics

DEC: diethyl carbonate

DMC: dimethyl carbonate

DME: dimethoxyethane

DOE: Department of Energy

EC: ethylene carbonate

ECHA: European Chemicals Agency

EDS: energy-dispersive x-ray spectroscopy

EEPS: engine exhaust particle sizers

EMC: ethyl methyl carbonate

EPA: Environmental Protection Agency

ERPG: Emergency Response Planning Guidelines

ESS: energy storage system

FM: Factory Mutual

FDS: Fire Dynamics Simulator

FEC: fractional effective concentration

FED: fractional effective dose

FID: flame ionization detection

FPRF: Fire Protection Research Foundation

FTIR: Fourier Transform infrared spectroscopy

GC: gas chromatography

GC-MS: gas chromatography mass spectroscopy

GC-TCD: gas chromatography thermal conductivity detector
HPIC: high-pressure ion chromatography
HRR: heat release rate
HRRPUA: heat release rate per unit area
ICC: International Code Council
ICEV: internal combustion engine vehicle
ICP-OES: inductively coupled plasma-optical emission spectrometry
ICP-MS: inductively coupled plasma mass spectrometry
IDLH: Immediately Dangerous to Life and Health
IFC: International Fire Code
IMC: International Mechanical Code
INERIS: National Institute for the Industrial Environment and Risks
kW: kilowatt
kWh: kilowatt-hour
LCO: lithium-cobalt
LEL: Lower Explosive Limit
LFL: Lower Flammability Limit
LFP: lithium-iron-phosphate
Li-ion: lithium-ion
LMO: lithium-manganese-oxide
LTO: lithium-titanium-oxide
MJ: megajoule
MLR: mass loss rate
MS: mass spectroscopy
MSS: micro-soot sensor
NCA: nickel-cobalt-aluminum
NDIR: non-dispersive infrared sensor
NFPA: National Fire Protection Association
NIOSH: National Institute for Occupational Safety and Health
NIST: National Institute of Standards and Technology
NLC: National Land Cover Database
NMC: nickel-manganese-cobalt
NOAEL: No Observed Adverse Effect Level
NOEL: No Observed Effect Level
OCV: open circuit voltage

OSHA: Occupational Safety & Health Administration

PACs: Protective Action Criteria for Chemicals

PAH: polycyclic aromatic hydrocarbons

PC: propylene carbonate

PCB: polychlorinated biphenyls

PCDD: polychlorinated dibenzo-p-dioxins

PCDD/F: polychlorinated dibenzo-p-dioxins and furans

PEL: Permissible Exposure Limit

PFAS: per- and polyfluoroalkyl substances

PM: particulate matter

PNEC: Predicted No-Effect Concentration

PTFE: polytetrafluoroethylene

ppm: parts per million

PU: polyurethane

PVC: polyvinyl chloride

PVdF: polyvinylidene fluoride

RISE: Research Institutes of Sweden

SBI: single burning item

SCC: Standards Council of Canada

SEM: scanning electron microscopy

SOC: state of charge

STP: standard pressure and temperature

TEEL: Temporary Emergency Exposure Limits

THR: total heat released

TR: thermal runaway

UL: Underwriters Laboratories

V: volt

VOC: volatile organic compound

Wh: watt-hour

Terms and Definitions

Battery: One or more cells connected together electrically in series, parallel, or both, to provide the required operating voltage and current levels [1].

Cell: The basic electrochemical unit, characterized by an anode and a cathode, used to receive, store, and deliver electrical energy [1].

Energy Storage Systems (ESS): One or more devices, assembled together, capable of storing energy to supply electrical energy at a future time [1].

Energy Storage System Unit: A permanent enclosure housing the components of the energy storage system which can be considered an *Energy Storage System Cabinet* or *Energy Storage System Walk-In Unit*.

Energy Storage System Cabinet. An enclosure containing components of the energy storage system where personnel cannot enter the enclosure other than reaching in to access components for maintenance purposes.

Energy Storage System Walk-In Unit. A structure containing energy storage systems that includes doors that provide walk-in access for personnel to maintain, test, and service the equipment and is typically used in outdoor and mobile energy storage system applications.

Exposure Limit Distance: The horizontal length, measured from the downwind edge of the BESS unit, at which toxic gas concentrations exceed thresholds for community (AEGL/ERPG/TEEL) or occupational exposure (IDLH).

AEGL-1 Distance: The horizontal length, measured from the downwind edge of the BESS unit, at which toxic gas concentrations exceed AEGL-1 thresholds.

IDLH Distance: The horizontal length, measured from the downwind edge of the BESS unit, at which toxic gas concentrations exceed IDLH thresholds.

Heavy Metals: An imprecise term often used as a group name for metals and semimetals (metalloids) based on categorization by density and/or that have been associated with contamination and potential toxicity or ecotoxicity [2].

Lithium-Ion Battery: A rechargeable storage battery that is composed of nonaqueous liquid or polymerized electrolytes, which provide ionic conductivity between lithiated positive active material electrically separated from metallic lithium or lithiated negative active material [1].

Lithium-ion Battery Fires: Combustion events in which components of a Li-ion cell, battery, or module are involved, whether the Li-ion cells were the source of ignition via thermal runaway, or not.

Module: A unit consisting of multiple cells connected electrically in series, parallel, or both, typically encapsulated with an outer casing and used in combination with other modules to provide the required operating voltage and current levels.

Off-Gassing: The event in which the cell case vents due to a rise in internal pressure of the cell [1].

Thermal Runaway: Self-heating of an electrochemical system in an uncontrollable fashion [1].

Flaming Thermal Runaway: Thermal runaway conditions in which off-gasses from the cells are ignited, via auto-ignition due to sufficient internal temperatures or via an external ignition source, and sustained combustion subsequently takes place. This condition is identified by the presence of visible flames.

Non-flaming Thermal Runaway: Thermal runaway conditions in which cells off-gas due to thermal decomposition but gases are not ignited, and no combustion occurs.

1. Introduction

1.1. Rationale

Over the past decade, there have been numerous thermal runaway events in outdoor, large-scale, lithium-ion (Li-ion) battery energy storage system (BESS) installations; however, quantification of the human health impact of these events has not been heavily investigated. Li-ion technology development and implementation has advanced ahead of comprehensive industry knowledge of hazards like thermal runaway events. Moreover, within the firefighter and first responder community, there are no standard methods for handling Li-ion thermal runaway incidents. Characterizing health impact allows firefighters and first responders to better respond to thermal runaway events, whether it be determining safe operating distances from the incident or issuing shelter-in-place and evacuation orders, as needed.

The primary objective of this research was to develop a methodology for characterization of the health impact of outdoor, large-scale, Li-ion BESS thermal runaway events. This was accomplished through fire and plume dispersion modeling based on data obtained from industry research and historical events. For the purposes of this research, a large-scale Li-ion BESS was defined as a utility or commercial or industrial scale Li-ion energy storage installation system. The primary research objective was accomplished through a literature review, plume dispersion modeling, and a risk analysis. The literature review served to identify and summarize the existing industry data on emissions and yields from Li-ion batteries during flaming and non-flaming thermal runaway. Plume dispersion modeling of Li-ion BESS thermal runaway events was performed, adjusted to various weather conditions. The findings from the literature review and modeling were used to conduct a risk assessment and gauge the impact of Li-ion BESS fires on human health. The findings from this research demonstrate a methodology that can be used in site-specific risk assessment and hazard mitigation analyses. The study findings related to exposure distances are specific to the modeled hazard scenarios and associated inputs; the relevant stakeholder or user should not blindly or blanketly apply the findings from the research in a hazard analysis without verifying that the modeled scenarios and associated inputs are applicable. This methodology is not meant to be conducted during an incident and will not be able to provide immediate results.

1.2. Approach

1.2.1. Literature Review of Lithium-ion BESS Fire Incidents

A literature review of peer-reviewed studies was conducted to identify a) the health and environmental impacts of large-scale Li-ion BESS thermal runaway incidents, b) factors controlling the degree of impact of large-scale Li-ion BESS thermal runaway incidents, and c) current modeling practices for modeling plume dispersion. Data was collected and analyzed to address the following questions:

- What gas yields are typical for large-scale Li-ion BESS thermal runaway events, and what factors influence them, e.g., cell chemistry?
- How are yields normalized, e.g., grams of gas per grams of fuel consumed, liters of gas per Watt hour (Wh)?

- How do plume constituents and yields differ for flaming and non-flaming thermal runaway events?
- What are representative heat release rates (HRR) and mass loss rates (MLR) for large scale Li-ion BESS units, and what is the typical duration of an event?

Findings from historical incidents that have occurred globally are also included. The 2021 Victoria Big Battery fire in Australia, the 2022 Moss Landing Li-ion battery fire in California, and the 2023 Queensland Li-ion battery fire in Australia, amongst others, were reviewed.

Data from Underwriters Laboratories, UL 9540A, Battery Energy Storage System (ESS) Test Method was also evaluated. Historical incidents and UL 9540A testing data were used to address the following questions:

- What are the specifications of the BESS systems involved in the incident, i.e., energy and power capacity, dimensions, fire suppression systems?
- What products of combustion were identified as a concern, if any, and how were they measured, e.g., air sampling of HF?
- How was the environmental and/or health impact quantified, e.g., measured concentrations compared to Occupational Safety and Health Administration (OSHA) permissible exposure limits (PEL)?
- What was the scale of the environmental and/or health impact of each fire, e.g., distance between source and impacted areas?
- What were the dominant controlling factors in incident outcomes and/or the severity of the health impacts, e.g., wind direction, wind speed, other weather conditions, plume dynamics, material burning?
- What firefighting tactics were implemented and how did they impact the environment and human health, e.g., spread of products of combustion through uncontained water sources?

The review of current modeling practices for modeling plume dispersion sought to address the following questions:

- What software and practices are typically used in plume modeling, and have they been validated?
- What are the required inputs, and what are the outputs?
- What are the limitations of each program?

The findings from the modeling review informed the model selection for the plume dispersion modeling.

1.2.2. Modeling BESS Plume Dispersion During Thermal Runaway

Modeling of plume dispersion, as the result of a thermal runaway event in a large-scale, outdoor Li-ion BESS installation, was performed to determine the impact of the plume on public health and the environment. The purpose of this task was to demonstrate how the methodology can be used by the relevant stakeholder or user to conduct a site-specific hazard assessment. Further, the modeling was performed to identify factors that should be considered when modeling a BESS fire. The modeled hazard scenarios involved a non-flaming and a flaming thermal runaway

event contained to a single BESS unit. The models included a bounding analysis for wind and temperature using minimum, average, and maximum conditions expected in areas of the country where BESS installations are most prevalent. Lithium-iron-phosphate (LFP) and nickel-manganese-cobalt (NMC) cell chemistries were evaluated. Associated HRR, MLR, and gas yields were determined using industry research data gathered in Task 1. Model outputs were analyzed to address the following questions:

- What are the concentrations of gases and particulates at various distances and heights, and for what duration?
- How do wind speed and ambient temperature conditions impact plume height and gas dispersion?
- How do flaming conditions and heat release rate impact plume behavior?

1.2.3. Analysis of Health and Environmental Impact

The analysis included reviewing the results of the plume dispersion models to determine the health and environmental impact of the modeled scenarios. The model results were analyzed to address the following questions:

- For protection of fire service personnel, at what distances, under various weather conditions, do gas concentrations exceed OSHA established Immediately Dangerous to Life or Health (IDLH) thresholds?
- For protection of the general public, at what distances, under various weather conditions, do gas concentrations exceed the U.S. Environmental Protection Agency (EPA) and/or industry established health thresholds?
- For protection of the environment, at what distances, do metal particulate concentrations, via deposition through the plume, exceed the EPA established environmental thresholds for different species?
- Is there a potential for significant environmental impacts from fire water run-off during a BESS thermal runaway event?

2. Background

The basic components of a Li-ion battery consist of an anode, cathode, separator, electrolyte, binder, and packaging or housing materials. Typically the binders consist of 2 to 5% of the total battery mass. Electrolyte makes up 8 to 18 % wt. The separator makes up 2 to 5% wt. The packaging and containment, which is usually composed of polyethylene or polyethylene terephthalate, makes up 3 to 25% wt.

The electrolyte typically consists of an organic solvent, a lithium salt, and a variety of additives [3]. Common organic solvents include ethylene carbonate (EC), diethyl carbonate (DEC), or dimethyl carbonate (DMC) and common lithium salts include hexafluorophosphate (LiPF_6), lithium tetrafluoroborate (LiBF_4), lithium hexafluoroarsenate (LiAsF_6), and lithium perchlorate (LiClO_4), with LiPF_6 being the most typical in commercial uses [3][4]. Regarding electrolyte additives, while thousands of variations have been tested and reported in the literature, these can be generally classified into groups based on their key elements, including boron-based, nitrogen-based, fluorine-based, silicon-based, phosphorous-based, sulfur-based, and dual salt systems [5].

The most established and typical binder material is polyvinylidene fluoride (PVdF) [3][4][6]. Other binder materials such as polyacrylonitrile, polytetrafluoroethylene (PTFE), styrene–butadiene rubber, carboxymethyl cellulose, and polyacrylic acid have been utilized to limited extents [6].

One of the main differences in Li-ion battery cells is the chemistry used for the cathode. Typical cathodes are composed of NMC, LFP, lithium-cobalt (LCO), nickel-cobalt-aluminum (NCA), and lithium manganese oxide (LMO) [7]. Other cathodes include lithium titanium oxide (LTO). Li-ion battery cells are composed of the housing, separator, electrolyte, cathode and anode foils, and the cathode and anode active materials.

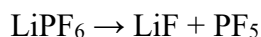
There are three typical types of Li-ion battery cells: pouch, cylindrical, and prismatic. Pouch cells are of flexible construction utilizing a metalized polymer film, cylindrical cells are constructed with a sealed aluminum “can” exterior, and prismatic cells are constructed with an aluminum casing in a rectangular shape [7].

Hill (2020) summarized thermal runaway of a Li-ion cell in open air into the following three stages:

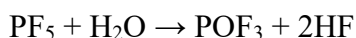
1. Due to voltage or temperature instability, the cell's internal temperature rises which causes gases to be emitted from the thermal decomposition of the electrolytes in the cell.
2. The voltage of the cell drops to zero and a direct internal short occurs with the anode and cathode, which initiates thermal runaway. Flames may or may not be present.
3. If sufficient oxygen is present, a secondary fire can occur because of the thermal runaway condition, resulting in the ignition of the surrounding battery materials such as electrolyte, polymers, and plastics [7].

Hill (2020) also described the gases released before, during, and after a thermal runaway event. Prior to thermal runaway, ethanol, and ethane, as well as other hydrocarbons are produced. During the thermal decomposition of the electrolyte, typically the effluent is a mixture of ethylene carbonate compounds and LiPF_6 . Gases produced during the “secondary fire” are like those of a fire involving typical plastics and include: H_2 , CO , HCl , HCN , and HF , as well as other hydrocarbons. Hill (2020) states that, generally, the composition of gases released during a thermal runaway event are similar across Li-ion cell chemistries, forms, and manufacturers, and the yield of gases can validly be assumed to be proportional to the electrolyte mass in the cell [7].

Most Li-ion battery cells utilize an electrolyte salt containing fluorine with the most common salt being lithium hexafluorophosphate (LiPF_6). When heated under dry conditions LiPF_6 will decompose into LiF and PF_5 .



However, in the presence of water, or humidity, the decomposition reactions include hydrogen fluoride and are as follows:



In comparing the quantities of HF produced by LFP cells and other cathode chemistries, the total HF produced has been found to be similar, despite the observation that other cathode chemistries, such as NMC/LMO, produce overall a much higher volume of gas, not limited to HF

[8]. This can be contributed to the greater production of hydrocarbon gases, such as CO and CO₂, which are influenced by the oxygen release of the decomposition of the NMC/LMO cathodes.

2.1. Industry Installation Standards

There are several standards for BESS design and installation, including NFPA 855 and Chapter 12 of the International Fire Code (IFC). NFPA 855 was first introduced in 2020 by the National Fire Protection Association (NFPA) and addresses the installation requirements for energy storage systems at certain capacities. Chapter 9 focuses on electrochemical energy storage systems (ESS), including systems utilizing Li-ion cells. The current version of NFPA 855 is the 2023 edition [9]. The IFC is developed and maintained by the International Code Council (ICC). Chapter 12 was added to the IFC in 2018 to address the installation, operation, maintenance, and decommissioning of energy systems. Section 1207 focuses on Li-ion BESS specifically. The current version of the IFC is the 2024 edition. The IFC defines Li-ion BESS as an ESS with capacity exceeding 20 kWh [10].

Chapter 9 of NFPA 855 requires that outdoor ESS installations must be listed to UL 9540, including Li-ion BESS systems. A fire code official approved hazard mitigation analysis must be completed for existing Li-ion BESS installation not listed with UL 9540. If the outdoor installation is located less than or at 100 feet from exposures, the total capacity of a Li-ion BESS installation cannot exceed 600 kWh. Locations that are “remote” (over 100 feet from exposures) may exceed 600 kWh in total capacity. NFPA 855 (2023)- Table 9.5.2 provides the relevant guidelines for the various components of an outdoor ESS. There are specific requirements for rooftop, garage, and mobile outdoor ESS installations, as well [9].

Fire suppression within outdoor walk-in units must be provided in accordance with Section 4.9, unless the installation is in a remote location and the ESS owner and fire code official agree that it is not required. Li-ion ESS, specifically, are required to have thermal runaway protection and explosion control in accordance with Sections 9.6.5.5 and 9.6.5.6. Thermal runaway protection must be evaluated as part of the UL 1973 or UL 9540 listing. The explosion control for Li-ion BESS walk-in units must include explosion prevention compliant with NFPA 69 or deflagration venting compliant with NFPA 68. However, explosion control is not required if approved by the fire code official based on a review of fire and explosion testing of the ESS, such as UL 9540A, and a deflagration hazard study has demonstrated that the flammable gas concentrations cannot exceed 25% Lower Flammability Limit (LFL). Fire and explosion testing, such as UL 9540A, must include evaluation of the deflagration mitigation measures integrated into the BESS [9].

IFC (2024) Section 1207 requires that all Li-ion BESS be UL 9540-listed. Enclosures must be made from noncombustible materials, and combustible materials cannot be stored inside ESS areas or units. Maximum enclosure size and separation requirements are provided in Section 1207. The maximum allowable capacity of a Li-ion BESS is 600 kWh; however, that quantity can be exceeded provided that a fire code official -approved hazard mitigation analysis and large-scale fire testing in accordance with UL 9540A are performed. The hazard mitigation analysis requires the following:

- “Fires will be contained within unoccupied ESS rooms or areas for the minimum duration of the fire resistance-rated separations identified in Section 1207.7.4.”
- “Fires involving ESS will allow occupants or the general public to evacuate to a safe location. (Material based on NFPA 855 2023 ed.)” [10]

If the outdoor installation is remote (over 100 feet from exposures), the maximum capacities for the whole system and individual units do not apply. The IFC provides Table 1207.8, which is similar to NFPA's Table 9.5.2. There are no significant differences between the applicable sections in NFPA 855 and Section 1207 of the IFC for outdoor installations. A hazardous exhaust system in accordance with Section 502.8 of the International Mechanical Code (IMC) must be provided if the ESS has the potential to release toxic gases during normal use conditions. This does not include release of toxic gases during abnormal or failure conditions, such as thermal runaway. Walk-in units must be protected by an automatic fire suppression system. Li-ion ESS, specifically, are required to have thermal runaway protection and explosion control complying with Section 911, unless explosion control is not required by the fire code official, based on UL 9540A testing [10].

Unlike NFPA 855, the IFC does not include a provision for existing Li-ion BESS with a fire code official-approved hazard mitigation analysis. Both the IFC and NFPA 855 include provisions for remediation and emergency response. Both codes require that ESS units can have a maximum capacity of 50 kWh and must be spaced a minimum of three feet apart unless the outdoor installation is remote. Smoke detection or radiant heat flux sensors in the area in accordance with NFPA 72 is required by both codes [9][10].

2.2. Common Thermal Runaway Quantification Methods

2.2.1. Heat Release

Heat release of Li-ion batteries can be quantified in several different ways. If the heat of combustion is known, mass loss can be measured and multiplied by the heat of combustion to calculate HRR. In cases of complete combustion, mass loss can calculate HRR with an error of less than 10%. For incomplete combustion, this method will overestimate HRR as CO production releases less energy than CO₂ production [11]. However, it can be difficult to use this method due to the unknown material composition.

Instead of calculating the heat of combustion for the Li-ion batteries, heat release is often quantified through oxygen consumption calorimetry. Oxygen consumption calorimetry calculates the heat release rate under the assumption that the heat of combustion per unit mass of consumed oxygen is approximately 13.1 kJ/g of O₂ [11]. Although the oxygen consumption method is widely used, it cannot capture the HRR during non-flaming thermal runaway and is more suited to combustion. The cone calorimeter, single burning item apparatus, and the Tewardson calorimeter typically utilize oxygen consumption calorimetry to measure heat release rate [12].

HRR can also be calculated through the ratio of CO and CO₂ mass produced. This method is called carbon dioxide generation calorimetry and relies on balancing the chemical reaction for incomplete combustion. The heat of combustion per unit mass of produced CO₂ is relatively constant at 13.3 kJ/g. The heat of combustion per unit mass of produced CO is also relatively constant at 11.1 kJ/g. The HRR can be calculated using the CO₂ or CO production rate [11]. This method has been favored over the oxygen consumption method for quantifying thermal runaway HRR because oxygen consumption does not account for the gases produced during thermal runaway. Additionally, oxygen consumption does not account for the variability of the Li-ion battery composition and its influence on stages of fire development [13]. The cone calorimeter and Tewardson apparatus can use carbon dioxide generation calorimetry [11].

Several common fire testing apparatuses include the cone calorimeter, single burning item (SBI) apparatus, Tewarson apparatus, and the accelerating rate calorimeter (ARC). The cone calorimeter is a bench-scale fire test designed to measure combustion characteristics of small samples. The sample is mounted on top of a load cell and heated by a cone-shaped radiator. The sample is open to the ambient atmosphere and gas is collected by an exhaust hood located above the sample and cone radiator [14]. The SBI is a medium-scale apparatus that was designed to characterize combustion characteristics of building products when exposed to a single burning item. The specimen is mounted on a trolley and positioned in an enclosure beneath an exhaust hood connected to the gas sampling system. The burning item is modeled by a 30-kW propane flame [15]. The fire propagation apparatus, otherwise known as the Tewarson apparatus, is a bench-scale fire test where the sample is mounted on a load cell and enclosed in a quartz tube that restricts the combustion area. The quartz tube is surrounded by four infrared heaters and attached to a hood connected to the gas sampling system [16]. The ARC is a bench-scale fire test designed to simulate a worst-case scenario where there is no heat exchange with the surroundings. The specimen is placed in a spherical vessel that is heated through a tube. The vessel is placed inside of an insulated containment vessel [17]. Mayonado et al. (2024) note that the fire testing method can cause variations in peak HRR data when testing the same specimen [12].

2.2.2. Constituent Quantification

This section describes several common methods to quantify toxic gases. Fourier Transform infrared spectroscopy (FTIR) is a technique used to identify organic, polymeric materials, and some inorganic materials through the measurement of infrared spectrum absorption and emissions. The spectrometer collects data over a wide spectral length and converts it to an infrared spectrum using the Fourier Transform. The different wavelengths in the spectrum correspond with different gases. This method is preferred over classic dispersive spectroscopy, as it can analyze multiple gases at once and the signal produced is stronger [18]. However, FTIR can underreport concentrations of reactive gases, such as HF, which can deposit out of the air before reaching the measurement equipment [8].

Non-dispersive infrared (NDIR) sensors are gas sensors consisting of a light source, detector and a filter allowing only infrared light to pass into the detector. The light is either absorbed or not absorbed by the gases. The Beer-Lambert law can then be used to calculate the wavelength of the detected infrared radiation. NDIR sensors are often used for measurements requiring high selectivity, sensitivity, and low power consumption. The absorption spectra of most volatile organic and inorganic gases of interest fall within the infrared spectrum, including CO, CO₂, NO, and NO₂. NDIR sensors are more inexpensive and simpler to operate compared to FTIR; however, NDIR sensors cannot analyze as many species at once [19].

Colorimetric gas detector tubes use a reagent to induce a color change in the tube when it interacts with the sample gas. Reagents vary depending on the specific gas that is being analyzed. A pump draws the sample gas into the tube, which is marked with concentration values. Colorimetric tubes are simple to operate, inexpensive, and portable. However, they are subject to error as two gases may cause a similar color change if they have similar properties [20]. Additionally, the concentration readings rely on visual indicators, which are more subjective.

Ion chromatography is a form of liquid chromatography that measures ions based on their interaction with resin. The sample is passed through the top of a pressurized column. Eluent, an

ion extraction liquid, is flowed top-down in the column to separate the sample into ions. Different ions will separate at different rates down the column. Retention time of each species is used to quantify concentration [21].

Gas chromatography is an analytical method in which the sample is dissolved in a solvent and vaporized to separate each species. A dry, inert, oxygen-free gas then carries the species through a heated column for quantification, usually through the effect of thermal conductivity on mass flow in a separation column. Gas chromatography can be paired with other gas quantification methods, such as gas chromatography mass spectroscopy (GC-MS), gas chromatography thermal conductivity detection (GC-TCD), and flame ionization detection (FID) [22]. Thermal desorption gas chromatography (TD-GC) is a method utilizing gas chromatography where the sample is concentrated on a sorbent. The sample is then released via heat and an inert gas flow into a GC-MS [23].

Mass spectroscopy (MS) quantifies gases based on mass to charge ratio. The sample is bombarded by electrons which ionize and fragment the sample. Ions are passed through a mass analyzer and sorted by mass to charge ratio. The relative peaks determine concentration. A common mass analyzer utilized in GC-MS is a quadrupole-ion trap analyzer. The quadrupole MS holds ions for long periods of time for analysis [22]. Inductively coupled plasma mass spectroscopy (ICP-MS) is a form of mass spectroscopy that separates the ions via plasma. A liquid sample is nebulized and transferred into argon plasma, which decomposes and ionizes the species [24]. Mass spectrometers can continuously scan and quantify gases; however, samples may thermally degrade before they reach the mass analyzer [22].

The operating principle of thermal conductivity detection (TCD) is measuring the change in the thermal conductivity of the carrier gas. The sensor contains an inlet, outlet, and a heating wire. The carrier gas and sample change the temperature of the heated wire upon entering. Thermal conductivity can be calculated from the temperature and resistance of the heated wire. Typically, the carrier gas will also be monitored by itself for calibration. TCDs are capable of analyzing both organic and inorganic species; however, it has lower sensitivity compared to other detection methods and a dependency on flow rate and concentration [22].

FID is a form of gas analysis method used to detect hydrocarbons. The detector provides little to no response for inorganics, CO, CO₂, and water. The FID burns a pure hydrogen flame. Below the flame, sample gas is introduced, mixed with H₂, and passed through the flame. This process removes the hydrogen from the sample gas via decomposition and then ionizes the remaining carbon. The carbon is counted using an electrometer [25].

Inductively coupled plasma optical emission spectroscopy (ICP-OES) quantifies gas ions by measuring the energy emitted by energized ions. Gases are ionized via argon plasma in the same process performed in ICP-MS. Energized ions emit photons until they return to their de-energized state. The photons have wavelengths that correspond to the species [26].

Scanning electron microscopy (SEM) uses a focused beam of electrons to scan a specimen for higher resolution images. This method is primarily utilized to characterize solid materials. SEM uses electrons instead of light because electrons have shorter wavelengths, which will produce a higher resolution. The electrons are accelerated via a specified accelerating voltage through lenses. SEM can be combined with energy-dispersive x-ray spectroscopy (EDS) to determine elemental composition of the sample. EDS utilizes the X-rays emitted from a sample during imaging to find elements associated with the energy differential [27].

3. Literature Review

The findings of the literature review are summarized below¹. Studies that were not available in English were excluded.

3.1. *Peer Reviewed Publications*

The first goal of the literature review was to identify thermal runaway characteristics of Li-ion batteries, including propagation rates, gas emission composition and yields, HRR, MLR, total heat released, total gas produced, and cell gas venting temperature. These characteristics were identified as they would be relevant for developing modeling inputs. How these characteristics varied between cell chemistry, state of charge (SOC), cell geometry, number of cells and their arrangement, cell capacity, and flaming or non-flaming conditions was also investigated. An internet search was utilized to identify literature that included the keywords “lithium-ion battery,” “thermal runaway,” “flaming,” “non-flaming,” “health impact,” “toxic gases,” “emissions yields,” and “BESS testing.” Publications that did not quantify the identified thermal runaway characteristics or identify the methods of quantification were excluded. The literature review primarily focused on determining characteristics for LFP and NMC cells. While some studies evaluated cell chemistries outside of LFP and NMC cells, that data was not considered for the modeling inputs. Studies on full-scale electric vehicles (EVs) were only included when they tested standalone batteries as well or used a method to isolate the contribution of the battery from the other vehicle components. A summary of all peer-reviewed publications is included in Appendix 7.1. Data from these studies was aggregated and is presented in Section 4.

3.2. *UL 9540A BESS Testing*

Data from industry testing of Li-ion thermal runaway was also included to identify thermal runaway characteristics and representative equipment parameters. UL 9540A, Test Method for Evaluating Thermal Runaway Fire Propagation in Battery Energy Storage Systems is a standard fire test that assesses thermal runaway, fire, and explosion behavior of a BESS at the cell, module, unit, and installation level. The current edition was published in 2019 by Underwriters Laboratories (UL) and is designated as an American National Standard by the American National Standard Institute (ANSI) and a National Standard of Canada by the Standards Council of Canada (SCC). The tests are performed progressively, i.e., if the BESS meets the requirements at a lower level, e.g., cell level, no further testing is required. The testing data is used to determine the required fire and explosion protection for the BESS installation [28].

Cell level testing is performed at 100% SOC after undergoing a minimum of two charge-discharge cycles at 100% SOC. The cell is placed inside a pressure vessel at atmospheric pressure with less than 1%vol of oxygen. Thermal runaway is initiated via flexible film heaters with a heating rate of 4 to 7 °C/min. The film heaters should cover as much of the cell case as possible. If the film heaters do not initiate thermal runaway, it is acceptable to use alternative heating methods or mechanical or electrical stresses. Cell surface temperature is measured using K-type

¹ The literature review reflects the most recent information available at the time the study task was completed. However, due to the rapid progression of Li-ion technology and continual release of new study results, there may be more recent scientific literature available at the time of this report’s publication that are not reflected here.

thermocouples to determine venting temperature and onset of thermal runaway. GC is used to measure for CO, CO₂, and total hydrocarbons and other gases requested for measurement. A sensor capable of measuring H₂ in excess of 30%vol is used. LFL is determined from the cell gas composition in accordance with ASTM E918 [28].

Module level testing is performed at 100% SOC after undergoing a minimum of two charge-discharge cycles at 100% SOC. The module should be placed on top of a noncombustible surface in the orientation of installation. The test is conducted under a smoke collection hood for gas collection. A sufficient number of cells are forced into thermal runaway to create cell-to-cell propagation within the module. The number of cells required for this condition can vary. Thermal runaway is initiated using the same methods for cell level testing. The chemical HRR is measured using oxygen consumption calorimetry with a paramagnetic oxygen analyzer, NDIR CO₂ and CO sensors, velocity probe, and K-type thermocouple. The velocity probe and thermocouple are also used to determine vent gas velocity and temperature. Vent gas composition is determined via FTIR or an equivalent gas analyzer. FID is used to detect THC content. Smoke release rate is calculated using light transmission measurements from a photo detector [28].

Unit level testing is conducted with BESS units at maximum operating SOC installed per manufacturer instructions. There is an initiating unit, where thermal runaway is initiated and adjacent target units that represent the installation spacing. Tests are conducted indoors, unless there are controls and certain environmental conditions. BESS units may be tested for indoor, outdoor, or rooftop/garage, residential or non-residential use, or floor-, wall-, or ground-mounted installations. Integral fire suppression systems are allowed, but electronic and software controls (i.e., battery management systems) are not permitted [28].

For indoor installations, the vent gas composition, THC content, chemical HRR, and smoke release rate measurement methods are the same as those used for module level testing. The gas data is compared to the smallest room installation specified by the manufacturer. Convective HRR is calculated using the relationship between exhaust flow rate, exhaust temperature, and specific heat. For BESS units installed in locations with combustible construction, wall surface temperature is measured. Schmidt-Boelter heat flux gauges and K-type thermocouples are used for heat flux and temperature measurements. Outdoor and rooftop/garage unit tests do not need to evaluate chemical and convective HRR, gas composition, temperature, and velocity, and smoke release rate if they will only be listed as outdoor use [28].

Installation level testing assesses fire and explosion mitigation methods for the BESS and is only intended for indoor, non-residential use. The effectiveness of sprinklers and the fire protection plan are assessed. A similar setup to the unit level test initiating and target units is used [28].

A Google Search was utilized to obtain UL 9540A test data for various Li-ion BESS manufacturers and models. These test reports were reviewed for applicable information on equipment composition and specifications, thermal runaway characteristics, fire behavior, and products of combustion. Tests were only included if they were performed at the unit level or if the cell and module level tests were associated with a unit level BESS. Furthermore, units had to be designed for an outdoor, ground-mounted installation. Tests were also excluded if the relevant product information, i.e., cell chemistry, capacity, were not available online.

3.2.1. Enphase IQ Battery 5P

The search found UL 9540A cell (Project Number: 4790222974), module (Project Number 4790222974), and unit (Project Number: 4790527540) level tests performed by UL. The reports were summarized by Enphase [29]; the original UL reports were not found. The IQ Battery 5P was certified for both indoor wall- or floor-mounted and outdoor wall- or ground-mounted installations.

The Enphase IQ Battery 5P is a BESS using LFP cell chemistry. It is rated for 5.0 kWh at 76.8V with a power rating of 3.84 kW. The unit is populated with a single module and cannot be connected to other units. The dimensions of the IQ Battery 5P are 0.98 m by 0.55 m by 0.188 m [30].

In the cell level testing, the vent gas composition was reported to be approximately 60.9% H₂, 17.4% CO₂, 6.9% CO, 4.5% methane, and 3.5% ethylene, along with various other hydrocarbons at less than 1% each. The test results showed that thermal runaway was induced in the cell, and the vent gas composition was flammable. As a result, the cell level testing did not pass the performance criteria; thus, module level testing was required [29].

In the module level testing, the modules were rated at 64.4 Ah at 76.8V and consisted of LFP type battery cells with a total module mass of 35 kg. There were 24 cells in the module connected in series. During the test, only smoke was observed. There were no flames, sparks, or flying debris. There was 937 L of total hydrocarbons, 543 L of CO₂, 47 L of CO, and 163 L of H₂ produced [29].

In the unit level testing, the initiating unit was populated with one module with the same specifications as those tested previously. Three target units were placed 3 to 6 feet away from the initiating unit. During the test, no external flaming, debris, or reignition were observed. There was 1,394 L of total hydrocarbons, 0.06 L of CO₂, 0.41 L of CO, and 251 L of H₂ produced [29].

3.2.2. Fortress Power eVault Max

The search found a UL 9540A unit (Project 80128223) level test performed by CCIC-CSA International Certification Co., Ltd. Kunshan Branch and Shanghai Huahui Testing Co., Ltd on a Fortress Power eVault Max [31]. The cell level testing (64.280.21.60315.01) was performed by TÜV SÜD New Energy Testing (Guangdong) Co., Ltd; however, the report was not found online. Module level testing was not performed. The eVault Max was tested for indoor floor-mounted installation, which is considered representative of outdoor ground-mounted installation.

The eVault Max uses LFP type cells. The individual unit is rated for 360 Ah at 51.2V (18.5 kWh) but can be scaled up to 370 kWh when combined with other units. The unit dimensions are 0.515 m by 0.515 m by 1.073 m and it has a total weight of 235 kg. The eVault Max holds four modules [32].

Unit level testing of the eVault Max was performed by CCIC-CSA and Shanghai Huahui Testing on May 18, 2022. No fire detection or suppression is provided in the unit. Film heaters were used to initiate thermal runaway in the second module from the bottom of the rack [31].

During the test, six cells underwent thermal runaway. Cells vented and released heavy smoke during thermal runaway. No flying debris or deflagration was observed. The test was terminated due to temperatures inside the modules returning to ambient. No flames were observed. Gases measured were O₂, CO, CO₂, H₂, and total hydrocarbons [31].

3.2.3. Samsung SDI Model PHR0000-004AE3D

The search found UL 9540A unit (Project Number: 4789231760) level tests performed by UL on a Samsung SDI Model PHR0000-004AE3D [33]. Summaries of the cell (Project Number: 4788881139) and module (Project Number: 4788881153) level testing were included in the unit level report. While only one model was tested, the Samsung SDI Model PHR0000-004AE3D is considered representative of the Samsung SDI Model PHR2383-001A. The Samsung PHR0000-004AE3D is designed for outdoor, ground-mounted installations.

The Samsung PHR0000-004AE3D is a metal rack frame without a door. The dimensions are 0.465 m in length, 1.392 m in width, and 2.690 m in height. The Li-ion cells utilized in the Samsung BESS are prismatic cells with a combination of NCA, NMC, and LMO chemistries. Each module has compressed epoxy sheet impregnated with Novec 1230 [33].

In the cell level testing performed by UL, the cells associated with the Samsung PHR0000-004AE3D were Model CS1000RT001A rated for capacity of 100 Ah with a nominal voltage of 3.8V and mass of 2100 grams. The cells were forced into thermal runaway via external temperature ramp heaters. The total cell gas volume was 240 L. The cell vent gas composition was reported to be approximately 39.6% H₂, 25.2% CO₂, 16.6% CO, and 18.7% total hydrocarbons. The test results showed that thermal runaway was induced in the cell, and the vent gas composition was flammable [33].

In the module level testing performed by UL, the modules were Model EM1762AL001A rated for capacity of 200 Ah with a nominal voltage of 88.32V and mass of 120 kg grams. The modules contained 48 of the previously tested cells in 24S2P format, i.e., 24 cells in series and 2 cells in parallel. Thermal runaway propagated through all cells in the module. External flaming and flying debris were observed; no reignition occurred. CO, CO₂, H₂, and hydrocarbons were not observed pre-flaming, and 20 L of CO and 800 L of hydrocarbons were produced after flaming. Peak heat release rate was 1,000 kW [33].

Unit level testing of the Samsung PHR0000-004AE3D was performed by UL on March 9, 2022. The unit was populated with the same modules as those tested in the module level testing, i.e., Samsung SDI, CS1000RT001A, combination NCA/NMC/LMO prismatic cells. The unit was populated with fourteen EM1762AL001A modules connected in series. The unit was rated for 247.3 kWh at 1236.5V. The equivalent BESS unit Samsung SDI Model PHR2383-001A has 27 modules and is rated for 238.5 kWh with an operating voltage of 1036.8 to 1344.6V. A cell in the third module from the bottom was forced into thermal runaway [33].

During the test, thermal runaway did not propagate from module-to-module or cell-to-cell. No external flaming or flying debris was observed and the peak HRR was below detectable limits. Cell venting was not observed. Approximately 80 L of hydrocarbons were produced, but CO, CO₂, and H₂ levels were below detectable limits. The peak smoke release rate was less than 1 m²/s and there was 262 m² of total smoke released [33].

3.2.4. Simpliphi BOSS 12 Cabinet

The search found summaries of UL 9540A module (AACD.E527394B) and unit (AACD.E527394C) level tests provided by Simpliphi Power on a Simpliphi BOSS 12 Cabinet [34]. Additionally, summaries of both tests were found on the UL database [35][36]. While only one model was tested, the Simpliphi BOSS 12 Cabinet is considered representative of the

Simpliphi BOSS 6 Cabinet. The Simpliphi BOSS 12 Cabinet was certified for both indoor and outdoor installation.

The Simpliphi BOSS 12 Cabinet is a BESS contained in a steel enclosure. The BOSS 12 is 0.75 m in length, 0.51 m in width, and 1.93 m in height, weighing 194 kg. The BOSS 6 Cabinet is 0.914 m in length, 0.406 m in width, and 0.914 m in height, weighing 81.64 kg. No fire protection systems are provided in the cabinet [37].

The BOSS 12 can fit up to twelve modules, while the BOSS 6 can fit up to six modules. The cabinets are compatible with several Simpliphi modules, including the AmpliPHI or PHI 3.8, 3.5, or 3.4 [37]. The Li-ion cells utilized in the BOSS cabinets are cylindrical, LFP cells [34].

Module level testing was completed for the PHI 3.8 battery module rated for 3.8 kWh at 48V. In this test, the modules consisted of 336, LFP type battery cells, arranged in 16S21P format. The total module mass is 35.5 kg [38]. Seven cells were forced into thermal runaway via film heaters. Only cell-to-cell propagation and smoke were observed. There were no flames, sparks, or flying debris. Levels of CO, CO₂, and H₂ were below the detectable limit. Approximately 1 L of hydrocarbons was produced [34][35].

Unit level testing of the BOSS 12 involved the same modules as those previously tested, i.e., Phi 3.8, LFP type battery cells. The unit was populated with 12 modules with a total capacity of 45.6 kWh. Thermal runaway was induced through simultaneous heating of 7 cells within a single module via film heaters. The module was the center module located in the row second from the bottom of the unit. During the test, there was no module-to-module propagation, flaming, flying debris, or smoke. Only cell-to-cell propagation was observed. As such, the smoke production rate and peak HRR were both 0. Gas composition was not reported [34][36].

3.3. *BESS Incident Case Studies*

The second goal of the literature review was to gather data on environmental and health impacts from actual BESS failure events, as well as typical event durations. An internet search was utilized to identify historical BESS thermal runaway and fire incidents and associated literature. The environmental impact quantification practices utilized for these incidents were identified, where applicable. The BESS incidents are summarized below in Table 1².

² The information presented on historical incidents reflects the most recent information available at the time the study task was completed. However, due to continued incidences of real-world thermal runaway events in BESS units, there may be more recent incidents at the time of this report's publication that are not reflected here.

Table 1. Historical BESS thermal runaway incidents.

Event	Conditions	Evac/Shelter in Place	BESS & Site Specs	Fire Cause & Spread	Air Monitoring	Water Monitoring	Soil Monitoring	Other Monitoring
McMicken (Surprise, AZ) [7]	Apr. 19, 2019 16:54 (explosion at 20:04) 83-94 F	-	LG Chem NMC Rack level runaway (2 MW, 10584 cells)	Cascading thermal runaway in single rack caused explosion	Air dispersion model: minimal impact (emissions not provided)	-	Surface and soil samples near fire site: chemicals of concern were undetectable/similar to control	-
Victoria, AUS [39]	July 30, 2021 10:00-16:00 23-35 mph N	Air quality warning (issued before taking air quality measurements)	212 Tesla MegaPacks NMC 300 MW/450 MWh	Liquid coolant caused arcing, wind pushed flames to 2nd MP	EPA (2 mobile stations w/in 2 km): good AQI ¹ (0-50) 2 hours post-fire extinguishment	Runoff firewater contained and analyzed, minimal environmental impact	-	-
Valley Center, CA [40]	Apr. 5, 2022 17:15-20:15 Low 50s to upper 60s No precipitation	-	LG Energy NMC 139 MW/560 MWh	Water cascade over single enclosure triggered by nearby prescribed burn	-	-	-	-
Elkhorn, CA [41]	Sept. 20, 2022 01:30-19:00 No wind until 2:30, 3-6 mph E-SE by 4 am No precipitation Upper 50-60 F	Shelter-in-place (issued before taking air quality measurements)	256 Tesla MegaPacks NMC	Single enclosure	EPA tested for fluoride and HF, no PM: good AQI ¹	-	-	-
East Hampton, NY [42]	May 31, 2023 ~10:00 to ~12:00 59-mid 60s F 6-8 mph SSE	Nearby road closures Railroad branch closure: reopened at 11:20	5 MW/40 MWh	Single enclosure	NYSERDA: air sampling inside BESS done on 6/14-16	DEC determined that groundwater sampling was unnecessary based	NYSERDA via project developer: Surficial soil and soil 1 foot below surface was collected on 10/4 from area that firewater ranoff to. Background levels collected from	NYSERDA: Surface sampling inside BESS on 6/14-16 and analyzed for heavy metals. No guidelines

		(issued before taking air quality measurements)				on soil sampling results	west and southeast sides. Concentrations below commercial NYSDEC Soil Cleanup Objectives or EPA Regional Screening Levels.	or reference samples were provided for comparison.
Warwick, NY (Bus Garage on County Road 1A near by Warwick Valley Central Schools) [42]	June 27 to July 29, 2023 65-68 F 6-12 mph SSE Heavy rain, high wind, power outages	Evacuation of school district: reopening 7/3 (issued before taking air quality measurements) Shelter-in-place (issued before taking air quality measurements)	6 Powin Energy 53' Centipedes LFP	Water leakage into multiple enclosures (no fire or thermal runaway propagation to other units) Alarms were triggered at a 2nd site (Church St) on 6/26 and 6/29 but no fire was detected	Industrial Hygiene Services and Air Quality: Air sampling performed on 6/28 while fire was burning, school located downwind. 0.1-0.5 ppm of CO and VOC outside. School indoor H2S below 0.2 ppm and CO and VOC were not detected. School indoor levels of PM2.5 were lower than outside.	-	-	Industrial Hygiene Services and Air Quality: surface sampling found no hazardous concentrations No lithium, bromide, or fluorine detected on any surface samples
Village of Chaumont, NY [42]	July 27 13:00 to August 1, 2023 11:00 mid 50s-70s F 12-17 mph max wind speeds Rain on July 27 and 30	Shelter-in-place: 1 mi lifted on Jul 27 at 21:00 (issued before taking air quality measurements)	General Electric NMC 4 discrete 5 MW BESS and one 2.5 MW BESS with 22.5 MW solar panel facility	Single enclosure	NYSERDA via OFPC: No readings except for maximum of 4 ppm HCN at the base of the container on 7/27. Low concentrations of CO and VOC (1 ppm) on 7/29. No readings on air monitors on 7/30. CO, VOC, and	NYSERDA: groundwater sampling from 11 drinking water wells. Samples were taken 8/4. Two wells had individual PAH levels exceed guidelines, but total PAH was acceptable. No other compounds exceeded	NYSERDA: surficial soil and bedrock samples taken at baseline and downwind locations. Samples were taken on 8/24. At SS-4, barium exceeded NYSDEC limits for commercial soil but not for groundwater soil. No other samples exceeded NYSDEC limits. No guidance on some compounds. One sample for SS-9 compounds not present in other sampling sites. Enclosures were removed on 11/14, samples directly beneath the	-

					HCN present only at the base of the enclosures on 8/1.	acceptable levels. The wells were resampled on 12/4, results have not been released.	enclosures were taken. Results have not been released.	
Valley Center, CA [43]	Sept. 18, 2023 17:15 6-7 mph W Upper 60s-70 F	Evacuation: 0.25 mi from 17:45 to 20:30 (issued before taking air quality measurements) Shelter-in-place: 0.5 mi (issued before taking air quality measurements)	LG Energy NMC 139 MW/560 MWh	Single enclosure	San Diego County: good air quality	San Diego County: good water quality	-	-
Bouldercombe (Queensland, AUS) [44][45]	Sept. 26, 2023 19:45 6-10 mph average N-NW	Shelter-in-place	40 Tesla MegaPack 2s 50 MW/100 MWh LFP	Failure on AC bus bar that propagated through modules in single enclosure	No fixed stations nearby FD monitoring showed good AQI ¹	-	-	-
Melba, ID [46]	Oct. 2 to 5, 2023	Evacuation, roads within a 200 ft radius were closed	Powin 2 MW/8 MWh	Water intrusion in a defective unit causing short circuit	Continuous 3 rd party monitoring from Oct 2 to 5 based on residential area location and winds	-	-	-

¹ A higher Air Quality Index (AQI) is associated with a lesser air quality and has the potential to result in negative health impacts. A range of 30 is considered a "good" AQI. A range of 151 to 200 is considered an "unhealthy" AQI. For more information on ranges, go to <https://www.airnow.gov/aqi/aqi-basics/>

The organizations responsible for air, soil, and water monitoring stated that there was little to no human and environmental health impact from the reviewed BESS incidents. The conclusions, however, must be put in context with some gaps in the testing methods. The McMicken, Victoria, Valley Center, and East Hampton incidents had no real-time air quality monitoring during the fire. Measurements were taken after the incident when the plume had already dispersed, making it difficult to ascertain the public impact during the event when gas production was highest. There was no water or soil quality monitoring for several incidents as well. When testing for environmental impact, some testing did not evaluate pollutants such as HF or other halogenated compounds, hydrocarbons, polycyclic aromatic hydrocarbons (PAH), per- and polyfluoroalkyl substances (PFAS), semi-volatile organic compounds, or VOC. Several incidents only analyzed AQI, which does not consider the impact of the aforementioned compounds. Furthermore, in some cases, it is unknown when and where monitoring was performed. In other cases, monitoring was performed well after the incident (e.g., East Hampton incident) with no consideration for weather-related impacts like precipitation that could dilute original contaminant concentrations in the soil. The lack of significant findings could indicate that either no significant contamination occurred or that contaminants were water soluble, biodegradable, and did not persist over time. As the monitoring results are inconclusive, this study aims to develop a methodology to better characterize the pollutant concentrations most relevant to human health and environmental impact.

3.4. Model Program Selection

The third goal of the literature review was to identify modeling programs and practices that could be used to characterize Li-ion thermal runaway health impacts. Google Scholar was utilized to identify literature that included the keywords “lithium-ion thermal runaway,” “fire modeling,” and “plume dispersion modeling.” Plume dispersion modeling was utilized to demonstrate how human health impacts could be characterized for a simulated thermal runaway event in an outdoor BESS installation. The modeling considered a thermal runaway event in a single unit that propagates without flaming, as well as a thermal runaway in a single unit that propagates with flaming. The selected scenarios were based upon failure modes reported in testing and real incidents. The objective of the modeling was to determine the concentrations of toxic gases contained in the fire plume at varying distances from the fire origin. The concentrations were compared against human health exposure limits to assess the potential impact on the surrounding population in the modeled scenario, and demonstrate a methodology that can be used in hazard evaluations.

The plume dispersion modeling program had to be capable of modeling both plume dispersion for the evaluation of health impacts and particulate deposition for the evaluation of environmental impacts. The program needed to simulate combustion from a point source over a short time scale (i.e., minutes) using inputs of emission yields and mass loss rate. In addition, the program had to model plume development close to the compartment and kilometers downwind to capture both the near and far-field impact. Table 2 provides a list of modeling programs assessed and their capabilities.

None of the programs listed below met all the identified requirements; therefore, two different models were chosen. Fire Dynamic Simulator (FDS) was chosen for fire modeling and to evaluate the health impacts of near-field plume dispersion. FDS is a computational fluid dynamics (CFD) model developed by the National Institute of Standards and Technology (NIST) fire modeling. It has been used by others to model BESS thermal runaway events [47], and is validated for plume

dispersion [48][49]. Models that were developed solely for a specific type of fire, e.g., wildfire propagation, pool fire, or jet fire, were excluded. While there are modeling programs that can model larger domains, the fire modeling was restricted to certain types of fires and did not allow for 3D modeling of the BESS unit. Pyrosim, a program developed by Thunderhead Engineering, was utilized as an interface for FDS during the modeling process. Smokeview, in conjunction with FDS and Pyrosim, was used to visualize the results.

While FDS is capable of soot deposition modeling, the algorithm was developed for deposition within a compartment and has not been validated for atmospheric deposition. Additionally, FDS is computationally expensive when modeling domains in the range of kilometers. Thus, AERMOD was chosen for far-field plume dispersion modeling and particulate deposition. AERMOD is a Gaussian plume dispersion model that has been extensively validated and is recommended by the EPA for plume dispersion modeling [50]. Other plume dispersion models were either cost-restrictive or not commercially available, were not capable of fine mesh sizes in meters, were not capable of inputting specific emissions yields, or did not include particulate deposition.

NOTE FOR USERS

While FDS and AERMOD were selected as the most appropriate models for this study, other models identified may be appropriate for a site-specific analysis, depending on the scope and objectives of the evaluation. The user should confirm which model(s) are the most suitable for their needs.

Table 2. Fire and plume dispersion modeling programs and their specifications.

Model Name	Domain (Cell Size)	Developed for?	Physics	Plume Modeling	Fire Modeling	Particulate Deposition	Emissions Inputs
FDS	m- ~1-2 km, computationally expensive at km (cm-m, multi-mesh)	Multiple plume and combustion scenarios, chemistry only for CO, may not predict unsteady dispersion well	TKE+LES (CFD)	Yes	Yes	Soot	Species mass loss rate
FLARE/ BUOYANT	Km (Determined automatically by CORINE, 100s m)	Forest or pool fire plumes, no phase changes in plume, no pollution, developed with HARMONIE (region locked to Finland)	Simple physics	Yes, can't handle vertical profiles well	Yes, simple	No	No
HIGRAD/ FIRETEC	~1 km, 100s ft to 10s mi. Computationally expensive (cm-m)	Wildfire- flame front, combustion	LES (CFD)	Yes	Yes, wildfire specific fuel combustion	No	No
WRF-SFIRE-CHEM	km or larger, landscape scale. Limited to 10 m above ground (10s m, multi-mesh)	Wildfire- atmospheric physics/chemistry, smoke & gaseous product transport, focus on fire propagation. CHEM for chemistry of emissions and yields. Dependent on WRF data	Eulerian Simplified combustion, focused on fireline/ atmosphere	Yes	Yes, Rothermel fire spread w/ prescribed fuel (can't input own fuel). No ignition point/fire history	No	No, emissions depend on pre-loaded fuel class
WFDS	~1 km, computationally expensive beyond 4 km (cm-m)	Wildfire- flame front, combustion, use WFDS-LS for fireline propagation	LES (CFD)	Yes	Yes	No	No, emissions depend on pre-loaded fuel class
ForeFire	-	Wildfire propagation, validated for large industrial fire	Simplified combustion focused on fireline propagation	No	Yes	No	No
FLACS	km (cm-m)	CFD, validated for flammable and toxic releases in industrial safety, explosion modeling	CFD	Yes	Yes	No	Yes, can specify fuel based on pre-loaded fuel class

PHAST	m (mm)	CFD, validated for accidental gas releases in industrial safety with add-ons for explosion, pool fires, and jet fires	UDM, CFD	Yes	Yes, pool and jet fire only	No	Yes, can specify fuel based on pre-loaded fuel class
AERMOD	-	Atmospheric dispersion does not handle low/complex wind speeds well. No aerosol dynamics. Uses weather station readings. EPA recommended	Gaussian	Yes, steady state	No, input point source with yields	Wet and dry deposition	Species mass loss rate
Meso-NH	10s m-km, micro & mesoscale (10s-100s m, multi-mesh)	Atmospheric physics/chemistry, has surface to atmosphere interactions, reliant on NWP databases (primarily European region locked)	TKE+LES	Yes, turbulence clarity sacrificed at coarser grid	Yes, coupled with ForeFire	Dry deposition of aerosols, dust and sea salt	Based on deposition velocity
Fluidyn PANACHE/ PANEP module	10s m (m) Time scale in hours-days	Gas dispersion, phase change, density/temperature. Can calculate ingestion dose of deposited pollutants	RANS, (CFD)	No	No, input mass flow rates	Wet and dry deposition	Yield based
ADMS	Up to 50 km (Up to 3000 grid cells)	Atmospheric dispersion, doesn't work well at low/complex wind speeds. Averaged concentrations	Quasi-Gaussian	Yes, Lagrangian plume model	No, input point source with yields	Wet and dry deposition	No
CALPUFF	Up to 1000 km	Atmospheric dispersion, good in light wind conditions, PM modeling	Puff model, unsteady	No	No, input buoyant and line sources (no point)	Wet and dry deposition	Yes
ANSYS Fluent	km (m)	Fluid dynamics with 3D modeling	RANS steady, unsteady LES (CFD)	Yes	No, input point source with yields	No	No
CHIMERE	km, anything below 1 km is parameterized (10s km)	Atmospheric dispersion modeling with chemistry, PM tracking, large time steps (order of 0.5 days+)	-	Yes, no convection modeling over heat source	No	Natural emissions (biomass/ sea salt/ mineral dust)	No

WRF-CMAQ	km to 100s of km via nested domains	Vertical diffusion and transport with aerosol and gas-phase chemistry. Couples CMAQ for plume and WRF for weather	Eulerian conservation of mass	Yes	No	Wet and dry deposition	Yes
Unified Forecast System Aerosol	1000s of km	Earth Systems modeling including short range weather and air quality, currently an ongoing project	-	Combination of FV3, CCPP, JEDI, Noah-MP LSM, MOM6, CICE6, WAVEWATCH III, GOCART	-	-	-
ALOHA	100s of km	Accidental and volatile release of flammable chemicals	Gaussian and Heavy Gas models	Yes, can model individual species release of toxic vapors	Yes, pool fires, BLEVEs, vapor cloud explosions, jet fire, flammable clouds	No	Yes, has own chemical database

4. Risk Assessment Methodology

4.1. Thermal Runaway and Plume Dispersion Modeling

The modeled scenario involved a 3.101 MWh outdoor BESS unit undergoing thermal runaway in a rural area with flat terrain and low-lying vegetation. It was assumed that there were no surrounding buildings or complex terrain. Non-flaming and flaming thermal runaway scenarios³ were modeled with both LFP and NMC cell chemistry. No fire suppression was modeled.

A bounding analysis on wind and temperature was conducted to determine the impact of meteorological conditions on plume dispersion in FDS/Pyrosim. No precipitation or variation in relative humidity was modeled. In addition, 0 m/s wind scenarios were run in FDS/Pyrosim with an ambient temperature of 22°C to provide the baseline toxic gas concentrations in the plume. For AERMOD, an identical reference set of meteorological conditions was used to run all simulations; therefore, the impact of varying meteorological conditions was not assessed, only the cell chemistry and thermal runaway conditions.

NOTE FOR USERS

While the conditions simulated in the models do not account for all possible factors, they serve as a basic scenario to identify relevant factors and develop a modeling approach for outdoor, large-scale, Li-ion BESS thermal runaway incidents. For a given project, the modeled scenario should be based on reasonably expected site conditions and feasible BESS failure scenarios for the subject equipment installation.

4.1.1. Fire Dynamics Simulator and Pyrosim

For all simulations, a generic BESS unit was utilized. The unit consisted of a steel enclosure with a length of 7.25 m, a width of 1.63 m, and a height of 2.51 m. The enclosure consisted of six full battery bays, one control bay, and one shared battery and control bay. All bays were separated by vertical metal panels but contained vent openings to an interstitial space at the top of the enclosure. This interstitial space contained a vent opening to the exterior on the front face of the unit. Each full battery bay contained three modules, and the shared battery and control bay contained one module. Each module contained 336 prismatic cells, for a total of 6,384 cells within the unit.

NOTE FOR USERS

In a site-specific analysis, the equipment configuration should be based on the BESS unit(s) that is, or will be, installed. This includes, but is not limited to, unit energy capacity, physical dimensions, mass of components, bay separation, vents, and cell and module type, quantities, and arrangement.

Figure 1, Figure 2, and Figure 3 present the isometric and front views of the BESS unit modeled in Pyrosim. The front wall was hidden to show the inside structure and module layout of the unit.

³ While real-world incidents can transition back and forth from non-flaming conditions to flaming conditions, the impacts of such an incident would be expected to fall within the bounds of modeled flaming only and non-flaming only scenarios.

In Figure 1 and Figure 2, the separation between the modules and interstitial space and the vent were hidden. Each grey block represents a module containing Li-ion cells. Non-flaming thermal runaway was modeled via species gas injection through vents located on the modules. Flaming thermal runaway was modeled by splitting combustion from the species gas injection. The combustion reaction was a simple reaction with fast chemistry. The modeled fuels were methane and H_2 , which are commonly produced in Li-ion thermal runaway. The radiative fraction of methane was set to 0.2. Toxic gases that were not associated with combustion were injected via vents. The red rectangles on top of the modules are the burner vents modeling combustion. The green rectangles on top of the modules are the supply vents modeling toxic gas release. In the non-flaming simulations, the combustion vents were removed, and only three gas burner vents, all located within the same battery bay, were left in place.

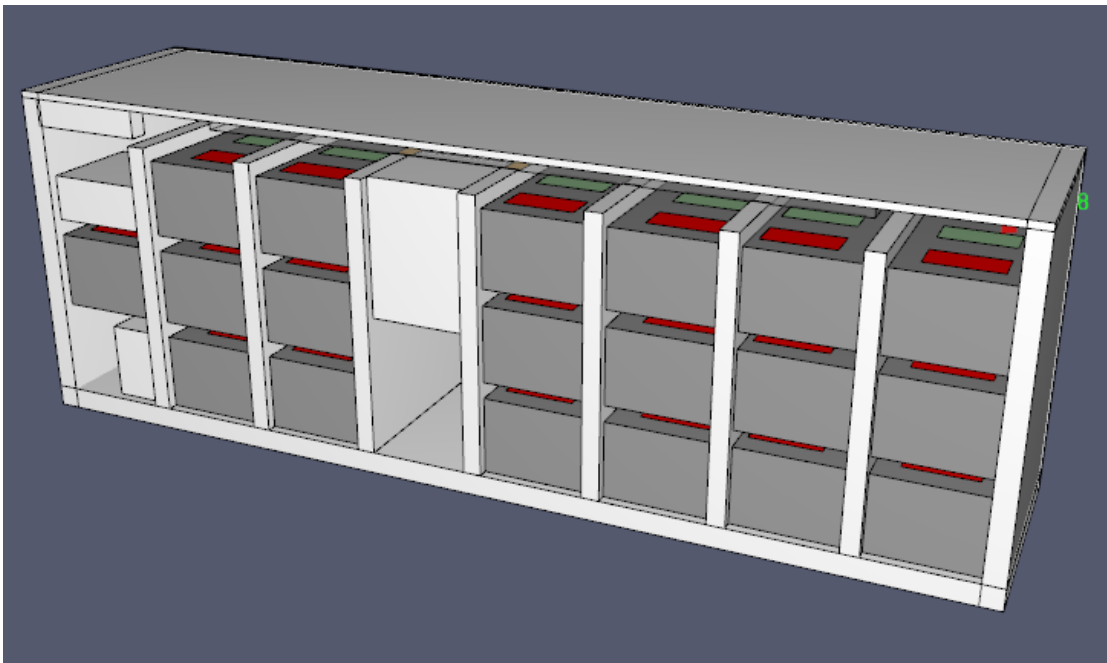


Figure 1. Isometric view of the Pyrosim model of the flaming BESS unit.

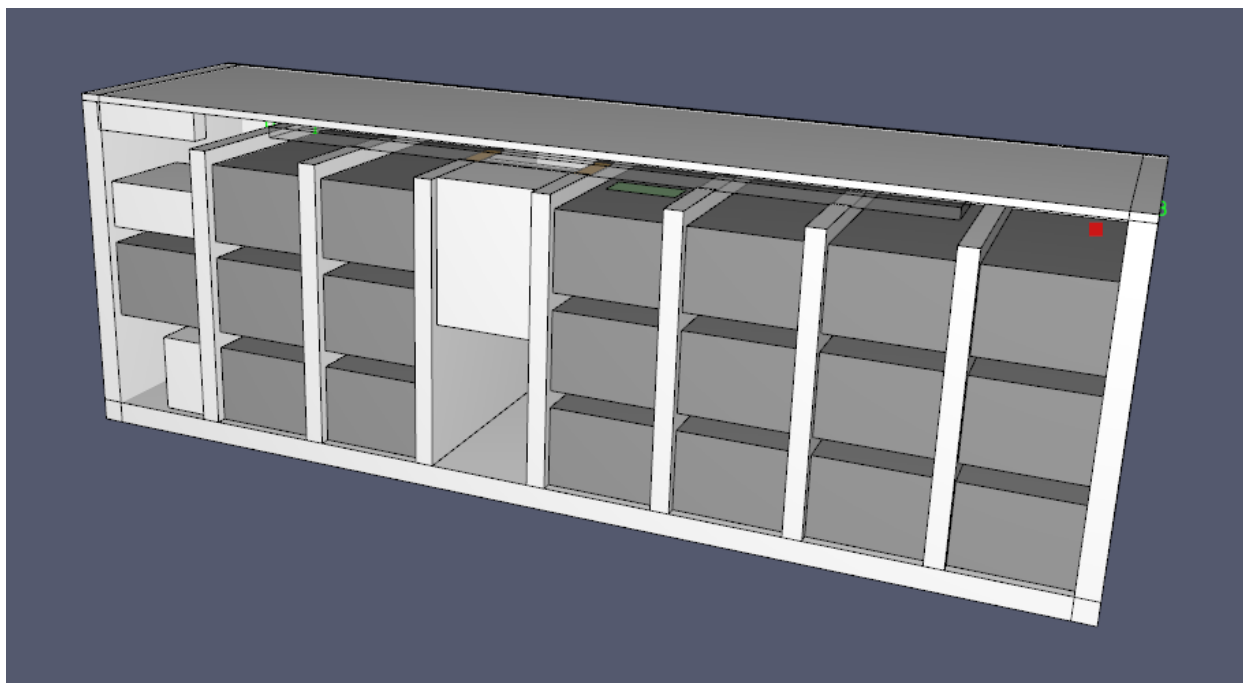


Figure 2. Isometric view of the Pyrosim model of the non-flaming BESS unit.



Figure 3. Front view of the Pyrosim model of the BESS unit.

User defined inputs in the FDS model included computational domain, ambient temperature, wind velocity, MLR, fuel, gas emission factors, and gas temperature. Modeling was limited to several hundred meters downwind of the BESS unit due to the computational expense of running a larger-scale simulation. The width of the computational domain was 32 m for all scenarios to encompass the full width of the plume. Model iterations were run to determine where HF fell below community exposure limits, and this was used to define the length and height of the domain. HF was used as the guiding factor for domain size because it has been identified as a unique

gaseous hazard to Li-ion battery thermal events. Computational domain dimensions are provided in Table 3.

Table 3. FDS computational domain dimensions.

Thermal Runaway Conditions	Width [m]	Length [m]	Height [m]
Flaming	32	100	43
Non-flaming		200	26

Cells containing the BESS unit were set to 0.125 m and gradually expanded to 0.25 m and 0.5 m cells. All cells were uniform. For the large eddy simulation code used in FDS, the grid can be resolved by dividing the characteristic length by cell size to find the number of cells along the characteristic length. There should be at least 10 cells along the characteristic length for good resolution [51]. For the flaming thermal runaway, the fire was contained to the 0.125 m and 0.25 m cells. The length of the fire was approximately the length of the BESS unit, so the characteristic length scale is approximately 7 meters. At the largest cell size (0.25 m), there are 28 cells, i.e., greater than 10 cells, along the length of the fire which provides an adequate grid resolution. Additionally, cell sizes were validated using the FDS Mesh size calculator [52]. The maximum HRR for a flaming thermal runaway scenario (24,980 kW) was used as the reference fire. The FDS mesh size calculator determined that the coarse, medium, and fine mesh dimensions should be 0.87 m, 0.35 m, and 0.22 m, respectively. The coarse, medium, and fine mesh sizes have smaller dimensions than the recommended cell sizes and would provide a higher resolution than necessary. Figure 4 and Figure 5 show the cell size expansion around the modeled BESS unit from the X-Y and Y-Z plane in Smokeview.

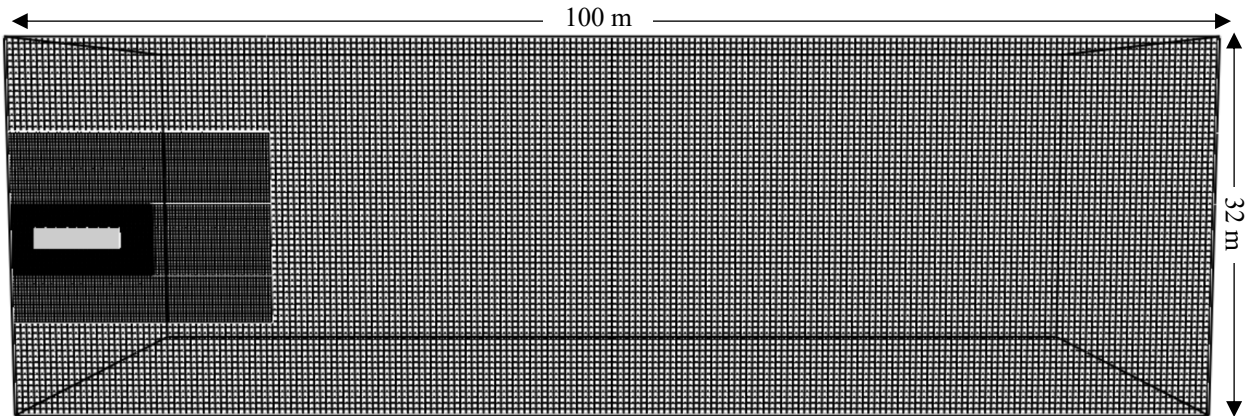


Figure 4. FDS cell sizes in the X-Y plane.

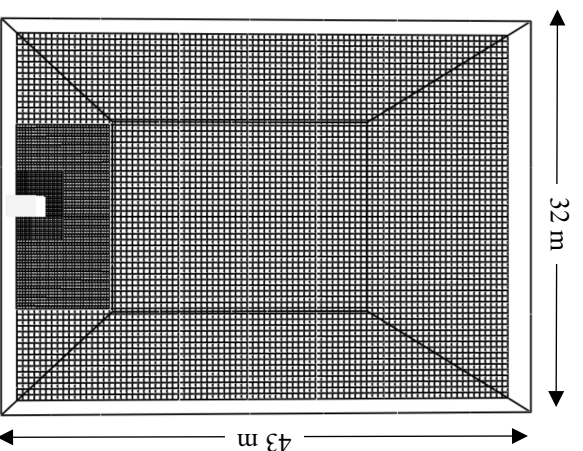


Figure 5. FDS cell sizes in the Y-Z plane.

All simulations were modeled with open mesh boundaries to allow for wind and smoke to pass through the domain boundaries. Wind effects were constant throughout the simulation duration, i.e. the wind speed did not increase or decrease and wind direction did not change. Ambient temperature was constant. Unless explicitly stated, default parameters in FDS were utilized.

The model simulations were run using cloud computing. Each simulation required 32 CPU cores with 1 Gb of RAM per CPU. The flaming simulations took approximately 6 to 13 hours to run, while the non-flaming simulations took approximately 3 to 16 hours. The total computational time ranged from 192 to 416 hours for the flaming simulations and 96 to 512 hours for the non-flaming simulations.

4.1.2. AERMOD View

Unlike FDS and Pyrosim, AERMOD View does not require a model of the BESS unit, nor does it require the fuel composition. User defined inputs in the AERMOD model included computational domain, weather station meteorological readings, emission rate in mass flux, pollutant identity, receptor grid and height, averaging period, and terrain. The plume from the BESS unit was modeled as a point source releasing the plume constituents at specified parameters informed by the literature data and/or the FDS simulation outputs.

All gases, except for NO_2 and SO_2 , were modeled in multichemical mode, which allows the user to specify individual mass flux rates for each species. Multichemical mode does not allow modeling of constituents with special dispersion algorithms. NO_2 and SO_2 have different dispersion algorithms compared to the generic gas dispersion model in AERMOD, so they were each modeled separately. Additionally, the particulate matter was modeled separately to utilize the deposition algorithm.

AERMOD calculates concentration and deposition at the user-specified receptors. The receptor grid had cells spaced at 5 m x 5 m in a computational domain of 5 km by 5 km with the BESS unit in the center. Iterations of the model were run to determine where the plume constituents fell below community exposure limits, and this was used to define the length and height of the domain.

Receptors were set to a height of 1.5 m for the simulations evaluating gases. Receptors were set to a height of 0 m for simulations evaluating particulate matter. The terrain was set to flat to eliminate contributions from complex topography or buildings.

NOTE FOR USERS

The flat terrain option should not be applied to all scenarios blindly. The user can use AERSURFACE to process land cover for surface characteristics and AERMAP to process elevation. AERSURFACE uses data from the National Land Cover Database (NLCD), which classifies land cover into water, developed, barren, forest, shrubland, herbaceous, planted/cultivated, and wetlands. These categories are further divided into subcategories for specific use. The user should assess the location at which the BESS unit is located and apply the relevant NLCD data.

4.2. Gas Production and Mass Loss Rate

To calculate gas concentrations, the release rates at the source must first be identified. To quantify the release of specific species during combustion, the MLR, which is dependent on HRR and the heat of combustion, must be estimated. Data from the literature review was used to estimate HRR and heat of combustion values, and subsequently MLR values, for the flaming model scenarios. An average, steady state MLR was modeled for each scenario and gas production rates were determined based on yield data obtained from the literature review. In the case of non-flaming thermal runaway, gas production is a result of thermal decomposition of the cell's internal chemistry, which is different from combustion, as it is typically defined⁴. The heat of combustion describes the heat energy released during combustion and hence is not useful in predicting the MLR of a material undergoing thermal decomposition. As such, a different approach was required to predict the rate of gases produced in the non-flaming scenarios. In these cases, the rate of gas released was estimated based on total gas volume production. An average, steady state gas volume release was modeled for each scenario and gas production rates for specific species were determined based on percentage gas composition data obtained from the literature review. It was noted, for both flaming and non-flaming scenarios, that average gas production rates do not capture peak gas production values, and as such, the peak values would not be considered in the health impact evaluation. However, the peak MLR and peak gas volume release rates are dependent on specific cell/module/unit configurations, cell geometry, failure mechanisms, ignition location, etc., and are thus difficult to predict. Additionally, peaks in a large-scale BESS unit will likely last on the order of minutes but community exposure limits are evaluated on the magnitude of minutes to hours. It is expected that community exposure will span time periods which include peaks and valleys in the MLR or gas production rate profiles. As such, it was determined that the use of the average gas production rates was considered the most representative approach⁵. Calculations for the average gas production rates in non-flaming and flaming scenarios are described below.

⁴ Thermal decomposition involves the breakdown of a compound into smaller constituents in the presence of heat alone. Combustion involves a reaction between a fuel and oxygen that produces heat and light, e.g., a flame.

⁵ If more specific data is available to the relevant stakeholder or user that allows for an accurate prediction of a peak MLR or peak gas production rate, and this peak is sustained for enough time to cause an increase in exposure risk, this could be used to produce more conservative results.

NOTE FOR USERS

If reliable experimental testing results for HRR, heat of combustion, MLR, and gas production are available for a specific BESS unit that is being evaluated, an approach based on observed HRR/MLR or gas release rate curves (i.e., non-steady state) could be considered. If such an approach is utilized, it is important to gather model inputs over a period that is in congruent with the exposure duration being utilized for health impact evaluation (i.e., 60 min exposure); using instantaneous peak values would likely lead to unrealistic results.

4.2.1. Non-Flaming Scenario

For the non-flaming simulations, calculations were performed assuming consumption of only one bay (nine modules) in the BESS unit. The total capacity of the consumed modules was 0.49 MWh. Thermal runaway propagation is dependent on heat transfer between adjacent modules [53]. Huang et al. (2020) showed that heat transfer in Li-ion battery modules is primarily driven by radiation and conduction through the connections between Li-ion cells [54]. In a non-flaming scenario, modules will release less heat due to the lack of flames. In the modeled configuration, the bays are separated by steel walls, which would further hinder thermal runaway propagation between bays. It is expected that the other bays would not experience enough heat transfer to initiate thermal runaway, hence, the modeled scenario is considered to be worst case.

NOTE FOR USERS

This scenario is specific to the BESS unit that was modeled. When evaluating specific BESS units, the user must analyze the specific unit to determine the feasible thermal runaway scenarios.

Based on the review of available literature, non-flaming thermal runaway does not produce HRR as there is no oxygen consumption from the flame [55]. To model mass loss from the cell off-gassing, data on total gas production normalized by capacity in Wh was used to estimate the total volume of gas produced from a single bay of cells. To estimate the gas release rate (L/s) for a non-flaming scenario, the predicted total gas production in L from the bay was divided across an estimated event duration.

Data on total gas production for non-flaming thermal runaway was found from the studies reviewed in Section 3.1. If capacity was not provided, a typical nominal voltage of 3.2 V for LFP cells and 3.6 V for NMC cells was assumed and used to calculate capacity from current. Sturk et al. (2019) measured HF quantities via both FTIR and gas-wash bottles. The gas-wash bottles were found to report approximately twice the amounts of HF than FTIR, due to treating all soluble fluorinated species as HF. As such, Sturk et al. (2019) suggested the gas-wash bottle method overpredicts HF quantities [8]. However, to be conservative, the average of the values measured via both methods, when provided by the study, are indicated in the tables below. Table 4 provides the total gas production and normalized total gas production per Wh for LFP cells.

Table 4. Total gas volume normalized by cell capacity for LFP cells.

Source	Cell Geometry	Total Gas Production [L]	Cell Capacity [Wh]	Total Gas Production [L/Wh]
Archibald (2021) [56]	Cylindrical	33.5	284	0.12
Gully (2019) [57]	Cylindrical	10.0	8	1.25
Gully (2019) [57]	Cylindrical	7.0	8	0.88
Gully (2019) [57]	Cylindrical	21.0	8	2.63
Gully (2019) [57]	Cylindrical	5.0	4.8	1.04
Gully (2019) [57]	Cylindrical	5.0	4.8	1.04
Golubkov (2014) [58]	Cylindrical	1.1	4	0.32
Golubkov (2015) [59]	Cylindrical	1.2	4	0.35
Golubkov (2015) [59]	Cylindrical	0.7	4	0.20
Golubkov (2015) [59]	Cylindrical	0.7	4	0.20
Golubkov (2015) [59]	Cylindrical	0.9	4	0.26
Golubkov (2015) [59]	Cylindrical	0.7	4	0.20
Golubkov (2015) [59]	Cylindrical	1.4	4	0.39
Golubkov (2015) [59]	Cylindrical	1.3	4	0.37
Proprietary Data ¹	Prismatic	97.2	502	0.19
Sturk (2019) [8]	Pouch	50.0	115.5	0.43
Yang (2022) [60]	Prismatic	232.7	715	0.33
Yuan (2020) [61]	Cylindrical	3.3	12.2	0.27
Yuan (2020) [61]	Cylindrical	3.8	12.2	0.31
Yuan (2020) [61]	Cylindrical	9.0	24.4	0.37
Yuan (2020) [61]	Cylindrical	11.7	36.6	0.32

¹ Data sourced from a proprietary testing report of a cells used in a commercial BESS.

The average total gas production normalized by capacity for LFP cells was 0.55 L/Wh. This number was multiplied by the capacity of the modules involved for a total LFP gas production of 269,000 L.

Table 5 provides the total gas production and normalized total gas production per Wh for NMC cells.

Table 5. Total gas volume normalized by cell capacity for NMC cells.

Source	Cell Geometry	Total Gas Production [L]	Cell Capacity [Wh]	Total Gas Production [L/Wh]
Amano (2023) ¹ [62]	Pouch	1.0	9.25	0.11
Amano (2023) ¹ [62]	Pouch	3.0	9.25	0.32
Amano (2023) ¹ [62]	Pouch	3.0	9.25	0.32
Archibald (2021) [56]	Prismatic	221.6	346	0.64
Bordes (2022) [63]	Pouch	37.7	70	0.54
Gully (2019) [57]	Pouch	458.0	226.8	2.02
Gully (2019) [57]	Pouch	223.0	226.8	0.98
Essl (2020a) [64]	Pouch	57.0	156	0.37
Essl (2020b) [65]	Pouch	94.0	216	0.44
Essl (2020b) [65]	Pouch	167.0	216	0.77
Essl (2020b) [65]	Pouch	103.0	216	0.48
Essl (2020b) [65]	Prismatic	94.0	216	0.44
Essl (2020b) [65]	Prismatic	159.0	216	0.74
Essl (2020b) [65]	Prismatic	106.0	216	0.49
Golubkov (2014) [58]	Cylindrical	5.9	10	0.60
Golubkov (2014) [58]	Cylindrical	3.3	6	0.59
Nedjalkov (2016) [66]	Pouch	200.0	172	1.16
Nedjalkov (2016) [66]	Pouch	85.8	172	0.47
Sturk (2019) [8]	Pouch	1500.0	287	5.23
Willstrand (2023) ¹ [67]	Prismatic	409.0	565.2	0.72
Willstrand (2023) ¹ [67]	Prismatic	332.4	565.2	0.59
Willstrand (2023) ¹ [67]	Prismatic	221.4	565.2	0.39
Willstrand (2023) ¹ [67]	Prismatic	113.0	565.2	0.20
Willstrand (2023) [67]	Prismatic	55.0	565.2	0.10
Yang (2022) [60]	Prismatic	88.5	215	0.41
Yang (2022) [60]	Prismatic	267.9	495	0.54
Yang (2022) [60]	Prismatic	454.6	710	0.64

¹ Average total gas production over tests conducted.

The average total gas production normalized by capacity for NMC cells was 0.76 L/Wh. This number was multiplied by the capacity of the consumed modules for a total NMC gas production of 372,000 L.

NOTE FOR USERS

The estimation of total gas production presented here utilized all available data, regardless of cell geometry, cell size, or cell/array/module configuration. Ideally, for a specific BESS unit, the total gas production estimates will be derived from experimental testing of the actual unit or unit components. However, in the absence of this, or as a supplement, the user should consider which literature data is most applicable. It may be necessary to filter data based on cell geometry, cell size, or cell/array/module configuration such that only the most representative studies are included.

Table 6 presents the times for peak gas venting to occur in large capacity (>100 Wh) LFP and NMC cells identified from the literature review. When finding average peak gas venting duration, only large capacity cells were considered as they represent the cells used in the modelled BESS unit. The cell capacity is expected to impact the duration of venting due to the higher gas production, so smaller cells were excluded.

Table 6. Peak cell venting duration for LFP and NMC large capacity cells (>100 Wh).

Source	Cell Chemistry	Cell Geometry	Peak Venting Time [s]
Archibald (2021) [56]	NMC	Prismatic	3.0
Essl et al. (2020a) [64]	NMC/LMO	Pouch	4.0
Essl et al. (2020b) [65]	NMC	Pouch	3.5
Essl et al. (2020b) [65]	NMC	Pouch	5.2
Essl et al. (2020b) [65]	NMC	Pouch	3.1
Essl et al. (2020b) [65]	NMC	Prismatic	2.0
Essl et al. (2020b) [65]	NMC	Prismatic	1.1
Essl et al. (2020b) [65]	NMC	Prismatic	11.5
Huang et al. (2021) [55]	LFP	Prismatic	229.8
Sturk et al. (2019) [8]	NMC	Pouch	21
Sturk et al. (2019) [8]	LFP	Pouch	300

Based on these values, the average peak venting time is 6 seconds for NMC cells and 265 seconds for LFP cells. The large difference in vent time is consistent with general findings of the literature review that show NMC cells experience a more violent failure at thermal runaway whereas LFP cells vent steadily over a longer duration.

To estimate cell propagation within the modules for a NMC cell scenario, it was assumed that, due to the very short vent duration, only one cell vents simultaneously. This results in a total event duration of 101 minutes for a single bay. To bound the analysis of this scenario, event durations of 0.5 hours and 2 hours were used. For an LFP cell scenario, assuming one cell venting at a time would result in a total event duration of 74 hours. However, due to the extended vent duration, it

is likely that multiple cells will vent simultaneously. Therefore, to gauge the impact of more catastrophic thermal runaway events, it was assumed that 10% of a module's cells vent simultaneously, or 11.2 cells. This results in a total event duration of 6.6 hours for a single bay. This is a conservative estimate compared to historical data which has shown that thermal runaway incidents, with limited flaming conditions, in LFP BESS units can continue for multiple days. For example, the Powin Energy BESS fire in Melba, ID [46] continued for over 3 days and the Powin Centipede BESS fire in Warwick, NY continued for at least 2 days [42]. In both incidents, thermal runaway propagated to multiple battery bays/compartments. To bound the analysis of this scenario, event durations of 6 hours and 12 hours were used. The resulting average gas release rates are provided in Table 7.

Table 7. Non-flaming average gas production rates for various durations.

Cell Chemistry	Duration [hr]	Average Gas Production Rate [L/s]
LFP	6	12
LFP	12	6
NMC	0.5	207
NMC	2	52

NOTE FOR USERS

When utilizing cell vent times to estimate propagation rates, it is important to consider the cell chemistry, geometry, and size and select the data that is most representative of the BESS unit being evaluated. Additionally, unit size, configuration, and composition will all effect the expected event duration. Ideally, for a specific BESS unit, the event durations utilized in the model will be based on large-scale testing of the equipment and/or historical incidents involving the same. However, in the absence of this, small-scale testing can be reasonably extrapolated. Thermal runaway propagation models can also be utilized to estimate propagation rates through the BESS unit, and thus total event duration.

4.2.2. Flaming Scenario

Unlike the non-flaming simulations, the calculations for the flaming simulations were performed under the assumption that all cells in the BESS unit would undergo thermal runaway. This scenario is based on the historical handling of flaming BESS thermal runaway events, as indicated in Section 3.3. It is common practice to let the BESS unit burn out, resulting in full consumption of all modules. Additionally, a flaming scenario is more likely to initiate thermal runaway propagation to the other modules due to convective and radiative heat transfer from the flames. Thus, it is expected that the full 3.101 MWh capacity of the modeled unit would be consumed in a flaming scenario.

NOTE FOR USERS

This scenario is specific to the BESS unit that was modeled. When evaluating specific BESS units, the user must analyze the specific unit to determine the feasible thermal runaway scenarios.

To estimate the HRR for a flaming scenario, the predicted total heat released (THR) from the unit was divided across an estimated event duration. Data on THR normalized by capacity in Wh for flaming thermal runaway was pulled from the studies reviewed in Section 3.1. If only THR was provided, it was normalized by the provided capacity or a nominal capacity calculated using a typical nominal voltage of 3.2 V for LFP cells and 3.6 V for NMC cells. Table 8 and Table 9 provide the normalized THR for LFP and NMC cells.

Table 8. THR normalized by capacity for LFP cells.

Source	Cell Geometry	THR [MJ]	Cell Capacity [Wh]	THR [kJ/Wh]
Andersson (2013) [18]	Pouch	6.8	112	61
Andersson (2013) [18]	Pouch	6.6	112	59
Andersson (2013) [18]	Pouch	7.1	112	64
Andersson (2013) [18]	Pouch	7.4	112	66
Andersson (2013) [18]	Pouch	7.5	112	67
Andersson (2013) [18]	Cylindrical	2.4	92	26
Ditch & Zeng (2020) [13]	Prismatic	143	5200	28
Ditch & Zeng (2020) [13]	Prismatic	1210	31200	39
Ditch & Zeng (2020) [13]	Prismatic	3810	83600	46
Larsson (2016) [68]	Cylindrical	2.8	92	30
Larsson (2016) [68]	Cylindrical	2.5	92	27
Larsson (2016) [68]	Cylindrical	6.6	132	50
Larsson (2017) ¹ [69]	Pouch	-	128	47
Larsson (2017) ¹ [69]	Pouch	-	112	70
Larsson (2017) ¹ [69]	Pouch	-	112	71
Larsson (2017) ¹ [69]	Cylindrical	-	92	30
Larsson (2017) ¹ [69]	Cylindrical	-	132	50
Liu (2020) [70]	Prismatic	1.7	70.4	25
Liu (2020) [70]	Prismatic	2.0	70.4	29
Liu (2020) [70]	Prismatic	2.4	70.4	34
Liu (2020) [70]	Prismatic	1.2	70.4	17
Liu (2021) [71]	Pouch	12.8	778	17
Liu (2021) [71]	Pouch	14.1	778	18
Liu (2021) [71]	Pouch	19.5	778	25
Meng (2020) [72]	Prismatic	2.1	81	26
Meng (2020) [72]	Prismatic	1.9	81	23
Meng (2020) [72]	Prismatic	1.3	81	16
Peng (2020) [73]	Pouch	6.7	219	30
Peng (2020) [73]	Pouch	6.4	219	29
Peng (2020) [73]	Pouch	5.6	219	26
Peng (2020) [73]	Pouch	4.2	219	19
Sturk (2015) [74]	Pouch	-	Varied	50
Sturk (2015) [74]	Pouch	-	Varied	62
Sturk (2015) [74]	Pouch	-	Varied	63
Sturk (2015) [74]	Pouch	-	Varied	61
Sturk (2015) [74]	Pouch	-	Varied	68

¹ Average THR over tests conducted.

Table 9. THR normalized by capacity for NMC cells.

Source	Cell Geometry	THR [MJ]	Cell Capacity [Wh]	THR [kJ/Wh]
Bordes (2022) [63]	Pouch	8	210	38
Bordes (2022) [63]	Pouch	10.5	210	50
Kang (2023) [75]	Pouch	1300	64092	20
Quant (2023) [76]	Unk	7.0	50000	16
Sturk (2015) [74]	Pouch	21.0	Varied	30
Sturk (2015) [74]	Pouch	5.0	Varied	28
Sturk (2015) [74]	Pouch	5.0	Varied	29
Sturk (2015) [74]	Pouch	1.1	Varied	29
Sturk (2015) [74]	Pouch	1.2	Varied	32
Willstrand (2020) [77]	Pouch	0.7	Varied	49

The THR normalized capacity has a wide range of values. To account for uncertainty and ensure that the mass loss rate is conservative, the average and positive standard deviation were calculated and added together to get the normalized THR values; 58.0 kJ/Wh for LFP cells and 43.5 kJ/Wh for NMC cells. The normalized THR was then multiplied by the maximum capacity of the BESS unit (3.101 MWh) to find a THR of 180,000 MJ for LFP cells and 135,000 MJ for NMC cells.

NOTE FOR USERS

The estimation of THR presented here utilized all available data, regardless of cell geometry, cell size, or cell/array/module configuration. Ideally, for a specific BESS unit, the THR estimates will be derived from experimental testing of the actual unit or unit components. However, in the absence of this, or as a supplement, the user should consider which literature data is most applicable. It may be necessary to filter data based on cell geometry, cell size, or cell/array/module configuration such that only the most representative studies are included.

Barowy et al. found that in full-scale testing on a BESS rack with NCA cells, it took approximately 20 minutes for flaming thermal runaway to propagate from the initiating rack to an adjacent rack. Thermal runaway then propagated from the first module in the adjacent bay to the top module over a period of 40 minutes. In total, it took 2.5 hours for thermal runaway to propagate to all modules [53]. Assuming a fire/thermal runaway starts in a center bay of the modeled unit, and assuming a similar horizontal propagation rate of 20 minutes from bay-to-bay, it would take at least 80 minutes for the event to propagate to modules in all 8 bays. Then, assuming the same vertical propagation time (40 minutes) for the entire rack of modules in a bay, the total time for all modules in the bay to become involved would be 120 minutes. This is still less than the total time for the test run by Barowy et al. (2021) [53], despite the rack in the test only having a total capacity 58 kWh, compared to the 3.101 MWh capacity on the modeled unit. Additionally, Ditch and Zeng (2020) found that flaming thermal runaway continued for 98 minutes and 160 minutes in single BESS racks with LFP cells and LNO/LMO cells, respectively [13]. Assuming the time for thermal runaway to propagate from the center module bay to the outer module bays is 80 mins, based on the results from Barowy et al. (2021) [53], utilizing the vertical propagation times (98-160 min) reported by Ditch and Zeng (2020) [13] produces total event times of 3 hours and 4 hours.

Therefore, use of a 2-hour incident duration for a flaming thermal runaway event was considered conservative, as the shorter the incident duration, the greater the MLR and gas production.

This is supported by the historical incident data which shows that for incidents where flaming thermal runaway occurred, in both NMC and LFP cells, the minimum incident duration was 2-hours. This occurred in the East Hampton incident, where the fire was contained by the enclosure's sprinkler system and therefore, it is expected the fire would have burned even longer if suppression had not been applied [42]. The Elkhorn and Victoria fires continued for durations of approximately 7.5 hours and 6 hours, respectively, and these events involved NMC cells [41][39]. Therefore, to account for a range of incident durations, flaming thermal runaway scenarios of 2, 4, and 6 hours were run. Evidence from the literature review indicates that LFP cells experience longer flaming thermal runaway durations [74], however, this was in the case of small modules (up to 10 cells). It is expected that once a full BESS unit becomes fully involved in a fire, the differences in propagation rates due to cell chemistry become negligible because of the high heat conditions and rapid flame spread. As such, the same incident durations were utilized for both NMC and LFP flaming scenarios.

NOTE FOR USERS

Unit size, configuration, and composition will all effect the expected event duration. Ideally, for a specific BESS unit, the event durations utilized in the model will be based on large-scale testing of the equipment and/or historical incidents involving the same. However, in the absence of this, small-scale testing can be reasonably extrapolated. Thermal runaway propagation models can also be utilized to estimate propagation rates through the BESS unit, and thus total event duration.

To calculate the average MLR, the average HRR was divided by heat of combustion. Data on heat of combustion in kJ/g for flaming thermal runaway was pulled from the studies reviewed in Section 3.1.

Table 10 provides the heat of combustion reported for LFP cell chemistries.

Table 10. Heat of combustion for LFP cells.

Source	Cell Geometry	Configuration	Δh_c [kJ/g]
Andersson (2013) [18]	Pouch	Cell	19.7
Andersson (2013) [18]	Pouch	Cell	19.4
Andersson (2013) [18]	Pouch	Cell	20.9
Andersson (2013) [18]	Pouch	Cell	20.8
Andersson (2013) [18]	Pouch	Cell	21.1
Andersson (2013) [18]	Cylindrical	Cell	16.6
Larsson (2016) [68]	Cylindrical	Module (9 cells)	19.1
Larsson (2016) [68]	Cylindrical	Module (9 cells)	16.1
Larsson (2016) [68]	Cylindrical	Module (5 cells)	16.3
Liu (2020) [70]	Prismatic	Cell	17.7
Liu (2020) [70]	Prismatic	Cell	18.2
Liu (2020) [70]	Prismatic	Cell	9.0
Liu (2021) [71]	Pouch	Array (2 cells)	13.7
Liu (2021) [71]	Pouch	Array (2 cells)	14.3
Liu (2021) [71]	Pouch	Array (2 cells)	17.2

The average heat of combustion for LFP cells was 17.3 kJ/g. Data on heat of combustion of NMC cells was limited; only one source was identified which found a heat of combustion of 46.4 kJ/g for a NMC battery pack. This value was noted to be significantly higher than what is found for LFP cells and is likely due to presence of additional plastics within the battery pack housing that were left in place during the test [75]. The tests indicated in Table 10 which reported values for LFP cells were conducted either on standalone cells or small groups of cells with limited other combustible materials. As such, these heats of combustion are more representative of the contributions by the Li-ion cells themselves. Viswanathan & Paiss (2020)⁶ reported a heat of combustion of 17.1 kJ/g for an NMC pouch cell based on UL 9540 test results [78]. This value is nearly identical to the average heat of combustion found for LFP cells; as such, the same heat of combustion was utilized for both NMC and LFP flaming scenarios. The resulting average HRRs and MLRs are provided in Table 11.

Table 11. Flaming average MLR for various durations.

Cell Chemistry	Duration [hr]	Average HRR [kW]	Average MLR [g/s]
LFP	2	24,980	1444
LFP	4	12,490	722
LFP	6	8,327	481
NMC	2	18,714	1082
NMC	4	9,357	541
NMC	6	6,238	361

⁶ Not included in this study's literature review due to not qualifying as a peer reviewed publication.

4.3. Toxic Gas Emissions

It is well understood that nearly all fuels, when burned, release chemicals and that the released constituents, if at a sufficient dose, can be harmful to human health. The types and concentrations of chemicals, i.e., emissions, are dictated by the chemical composition of the fuel and the burning conditions. It is not surprising that combustion of Li-ion batteries results in the release of chemicals with the same elements found in the fuel, e.g., fluoride; the conservation of mass necessitates that the same number of carbons, hydrogens, fluorides, etc. involved in the reaction will also be present as products of combustion. The literature review identified toxic and asphyxiant gases produced during Li-ion thermal runaway, including, but not limited to, benzene, CO, CO₂, HBr, HCl, HCN, HF, NH₃, NO₂, and SO₂. These gases were chosen for further evaluation in this study based on considerations of potential acute health effects, uniqueness to Li-ion battery fires, and availability of data.

Data on constituent gas yields was pulled from the peer reviewed studies identified in the literature review. The yield quantification methods used were a) species mass produced normalized by mass consumed in mg/g, b) percent gas volume composition, and c) species mass produced normalized by cell capacity in mg/Wh. The full list of yields can be found in Appendix 7.1. While some UL 9540A tests provided data on toxic gas yields, only the measurement of combustible gases is specified in the test procedures. The analysis methods for other gases are not prescribed and the tests results are not peer reviewed. As such, the UL 9540A gas yield data was not included in the yield calculations utilized for the models.

Model input yields were calculated by finding the average and positive standard deviation of the data points, then adding them together. If only one non-zero data point, e.g. yield was not found to be 0, was found for a constituent, it was excluded from review. For species with multiple non-zero data points and data points where the yield was 0, the 0 values were included when calculating the average and standard deviation.

It should be noted that the application of water may impact the production of certain toxic gases, particularly HF. Larsson et al. (2017) noted that the decomposition of LiPF₆ salt can be accelerated in the presence of water [69] and Andersson et al. (2013) noted that the application of water has the potential to shift the chemical kinetics of the thermal decomposition of LiPF₆ salt to favor HF production over POF₃ [18]. In support of this, Zhang et al. (2022) did find a notable increase in HF production when water cooling was applied [79]. However, in other experimental findings, Larsson et al. (2017) found that water application temporarily increased the rate of release of HF but did not have a significant impact on the total amount of HF released [69] and Andersson et al. (2013) found that the application of water mist did not impact the total amount of HF produced [18]. Another competing mechanism in the production of HF during a BESS incident where water is applied is the reactivity of HF with water. Cheng (2017) identified that water spraying has found to be an effective mitigation means for HF due to the tendency of HF gas to react with water molecules in the atmosphere, resulting in the transfer of fluorine from air to water [80]. As such, while the application of water could increase production of HF from Li-ion cells in some cases, the addition of water spray and mist may also reduce what is released into the atmosphere via air, though this would increase the presence of hydrofluoric acid in water runoff.

4.3.1. Non-Flaming Scenario

Mass production rate for each constituent was calculated utilizing the percent volume composition of gas constituents and the average total gas production rate found in Section 4.2.1. The percent volume for specific constituents, multiplied by the average total gas production rate, was then converted to mass using the ideal gas law under standard pressure and temperature (STP) or the provided reference temperature. STP was used when the gases were quantified after they had cooled to ambient temperature. Where percent volume composition was not available for a gas constituent, species mass production normalized by mass burned or by cell capacity in Wh was used to determine the total expected mass release of the constituent over the duration of the event. The total quantity was then divided by event duration to estimate an average mass production rate. Percent volume was prioritized over mass normalized by capacity, as it was applied as a ratio of the average total gas production rate; mass normalized by capacity has the potential to under- or overestimate the constituent to total volume ratio. Any chemicals that only had one non-zero data point were excluded from the evaluation.

Table 12 provides the species yields and mass production rates for the LFP non-flaming simulations. No data was found for HBr or SO₂. For NH₃, there were no percent volume data points and only one data point for mass produced normalized by mass burned or capacity, so it was excluded.

Table 12. Non-flaming species yields and mass production rates for LFP cells.

Species	Yield			Mass Production Rate [g/s]	
	%vol	mg/g	mg/Wh	6 hr	12 hr
Benzene	7.5	-	-	3.26	1.63
CO	14.6	-	-	2.28	1.14
CO ₂	66.7	-	-	16.34	8.17
HCl	1.9	-	-	0.39	0.19
HCN	0.5	-	-	0.08	0.04
HF	2.7	-	-	0.30	0.15
NO ₂	7.9	-	-	2.02	1.01

Table 13 provides the species yields and mass production rates for the NMC non-flaming simulations. No data was found for HBr for NMC non-flaming thermal runaway. There were zero percent volume data points for NH₃ and SO₂ and only one mass produced normalized by capacity data point for NH₃ in non-flaming NMC thermal runaway, so those constituents were excluded.

Table 13. Non-flaming species yields and mass production rates for NMC cells.

Species	Yield			Mass Production Rate [g/s]	
	%vol	mg/g	mg/Wh	0.5	2
Benzene	4.1	-	-	29.56	7.39
CO	38.7	-	-	100.04	25.01
CO ₂	44.8	-	-	181.97	45.59
HCl	0.2	-	-	0.67	0.17
HCN	-	-	0.02	0.01	0.01
HF	0.2	-	-	0.37	0.09
NO ₂	0	-	-	0	0

Toxic gas release was modeled as supply vents on three modules in one bay of the BESS unit. The species mass flux function was used to input gas production rates for individual species. Figure 2 shows the vent configuration of the non-flaming BESS unit.

In addition to the species mass production rates, FDS required inputs for gas temperature. The average gas temperature was pulled from non-flaming experiments and flaming experiments if the temperature was measured prior to ignition of the gases. Cell venting temperatures from flaming experiments where HRR contributed to an increase in temperature were excluded. The LFP cell venting temperature was calculated using values from Archibald (2021) [56] and Yuan et al. (2020) [61], resulting in an average temperature of 232°C. The NMC cell venting temperature was calculated using values from Bordes (2022) [63], Yuan et al. (2020) [61], and Zhang et al. (2019a) [81], resulting in an average temperature of 329°C.

NOTE FOR USERS

Vent gas temperatures are difficult to assess, and available experimental data was limited. While average vent gas temperatures have been identified based on this available data, it is expected that actual vent gas temperatures may be higher. Additional industry studies or equipment-specific testing is important in ensuring the accuracy of this critical parameter.

4.3.2. Flaming Scenario

Mass production rate for each constituent was calculated utilizing the species mass normalized by amount of mass consumed and the average MLR found in Section 0. Where yields normalized by mass consumed were not available, yields normalized by capacity were used. Yields normalized by mass consumed were prioritized over yields normalized by capacity due to the law of conservation of mass governing a more direct correlation between reactants and products. Yields normalized by mass burned or capacity were not available for particulate production, so a yield normalized by cell mass was utilized.

Table 14 provides the species yields and mass production rates for the flaming simulations. No data was found for HBr. There were no data points normalized by mass and only one data point normalized by capacity for HCN and benzene, so those constituents were excluded.

Table 14. Flaming species yields and mass production rates for LFP cells.

Species	Yield		Mass Production Rate [g/s]		
	mg/g	mg/Wh	2 hr	4 hr	6 hr
CO	35.1	-	50.7	25.3	16.9
CO ₂	1463	-	2112.5	1056.2	704.2
HCl	0.7	-	1.0	0.5	0.3
HF	24.8	-	35.8	17.9	11.9
NH ₃	0.5	-	0.7	0.4	0.2
NO ₂	1.9	-	2.7	1.4	0.9
SO ₂	3.5	-	5.1	2.5	1.7
Particulate	56 ¹	-	148.5	74.3	49.5

¹ Normalized by cell mass.

Table 15 provides the species yields and mass production rates for the flaming simulations. There were no data points normalized by mass and only one data point normalized by capacity for NH_3 , so it was excluded. While there was only one data point normalized by mass for HCl , it was prioritized over the yields normalized by capacity.

Table 15. Flaming species yields and mass production rates for NMC cells.

Species	Yield		Mass Production Rate [g/s]		
	mg/g	mg/Wh	2 hr	4 hr	6 hr
Benzene	-	145.5	62.7	31.3	20.9
CO	42.6	-	46.1	23	15.4
CO ₂	420	-	454.8	227.4	151.6
HBr	-	0.6	0.3	0.1	0.1
HCl	0.4	-	0.4	0.2	0.1
HCN	-	0.3	0.1	0.2	0.04
HF	8.2	-	8.9	4.4	3.0
NO ₂	-	4.5	1.9	1.0	0.6
SO ₂	-	17.7	7.6	3.8	2.5
Particulate	52 ¹	-	137.9	69	46

¹ Normalized by cell mass.

The flaming scenario was modeled using two separate vents, one for combustion products (CO , CO_2 , and soot) and the other for toxic gases. One of each vent was assigned to all nineteen modules. The toxic gas release was modeled using supply vents at the average non-flaming cell venting temperature found in Section 4.3.1. Combustion was modeled using burner vents with the average MLR found in Section 0. Figure 1 shows the configuration of the flaming BESS unit vents.

Because it is proprietary, the exact composition of chemical constituents in the combustible BESS cells and modules materials was not found in the literature and data searches. As such, a generic methane and H_2 mixture was utilized to model the fuel. Both gases are produced during Li-ion thermal runaway and are expected to ignite and contribute significantly to the combustion behavior. Additionally, methane burns cleanly without producing other constituents that could influence end concentrations. If only methane was burned, the incorrect yield for CO_2 would be produced. H_2 was added to produce the stoichiometry that would result in the required combustion yields.

The FDS combustion calculator [82] was utilized to calculate the ratio of methane to H_2 , as well as the yields for CO , CO_2 , and particulates required to produce the same yields found in Section 4.3. FDS accepts inputs for fuel ratio and yields for CO , soot, and HCN . The model then calculates a yield for CO_2 based on these inputs. The yields for particulates in LFP and NMC cells were inputted into the FDS model as soot. Calculations for HCN were not performed as it was assumed that the majority of HCN production would be due to the cell contents. To balance the mixture, percentages of methane were tested to find the correct inputs. The expected yield of CO_2 was then confirmed using the FDS combustion calculator. Table 16 and

Table 17 present the calculations for the percent methane in the fuel mixture, the required yield inputs for CO and particulate, and the CO_2 production calculated in FDS under those inputs.

Table 16. Combustion calculations for LFP cells.

Percentage Testing				
	CO	CO ₂	HCN	Particulate
Yield Required [kg/kg]	0.0351	1.4630	0.0000	0.1029
% methane	0.6900			
Inputs [kg/kg]	0.0509	-	0.0000	0.1491
Yield Calculated [kg/kg]	0.0509	2.1222	0.0000	0.1491
Yield if %fuel is burned [kg/kg]	0.0351	1.4643	0.0000	0.1029

Table 17. Combustion calculations for NMC cells.

Percentage Testing				
	CO	CO ₂	HCN	Particulate
Yield Required [kg/kg]	0.0426	0.4204	0.0000	0.1275
% methane	0.3600			
Inputs [kg/kg]	0.1183	-	0.0000	0.3541
Yield Calculated [kg/kg]	0.1183	1.1728	0.0000	0.3541
Yield if %fuel is burned [kg/kg]	0.0426	0.4222	0.0000	0.1275

Table 18 presents the final reaction inputs for the flaming thermal runaway combustion reaction.

Table 18. FDS combustion reaction inputs.

Chemistry	% methane	CO	Particulate
LFP	0.69	0.0509	0.1491
NMC	0.36	0.1183	0.3541

This ratio of methane to H₂ was released from the burner vent as fuel for combustion. AERMOD does not require the fuel composition to be identified, so this process was only utilized for FDS/Pyrosim.

4.4. Metal Emissions

The literature review identified the following metals can be emitted into the air during Li-ion thermal runaway: lithium (Li), nickel (Ni), manganese (Mn), cobalt (Co), aluminum (Al), copper (Cu), chromium (Cr), and zinc (Zn). Of these, only chromium and copper are typically considered heavy metals, however, all elements, including metals, can be considered toxic to the environment given a high enough dose [2]. Conversely, even heavy metals can be considered beneficial or essential to environmental health at low doses. For example, copper is considered an essential nutrient for some plant and animal functions and developments [83]. As such, each of these metals was examined further for potential environmental impacts.

The metal identified can be transported within the particulate matter produced during thermal runaway and deposited onto the surface with particulate that falls out of the plume. Therefore, it is important to predict the transport of metals within the smoke plume to assess the environmental impact to the surrounding area. Literature data on the particulate yield and percent mass composition of metals in the particulates produced from Li-ion battery thermal runaway was used to determine the AERMOD inputs. AERMOD requires inputs for particulate emission rate and size distribution to model total particulate deposition. The depositions of metals were calculated from the AERMOD model total particulate deposition outputs using the particulate composition.

4.4.1. Particulate Yields

Table 19 presents the particulate yields under non-flaming conditions identified from the literature review for particle sizes (0 to 900 μm) that can be expected to be transported out of the BESS unit enclosure and in the plume.

Table 19. Particulate yields for PM900 under non-flaming thermal runaway conditions.

Source	Chemistry	Mass/Cell Mass [mg/g]	Mass/Mass Lost [mg/g]
Wang et. al. (2020) [84]	NMC	16	NR
Wang et. al. (2023) [85]	LFP	55	NR
Zhang et. al. (2019a) [81]	NMC	47	NR
Zhang et. al. (2019b) ¹ [86]	NMC	48	170

¹ Study did not report specific quantities of PM for particle size ranges. Therefore, as a conservative approach, it is assumed all PM is PM500 or less.

Only one study reported yields in terms of particulate mass produced per mass of fuel lost. Therefore, to utilize the most data points, the yield in terms of mass of particulates produced per total mass of fuel was utilized in the model. Regarding NMC cells, the particulate yields from Zhang et al. (2019a) and (2019b) include PM10, which is the size at which particulate matter (PM) is respirable. However, they do not include PM2.9, as particles that size did not settle [81][86]. Wang et al. (2020) examined particle size distribution with a focus on PM500. The authors reported a size distribution of 0.005% for PM with a size of 0 to 30 μm [84]. Therefore, to conservatively account for the particles not quantified in experiments that looked only at settleable PM, a 1% increase was applied to the PM emission factors reported in Zhang et al. (2019a) and (2019b) [81][86]. Utilizing this methodology, the average PM emission yield is 37 ± 15 mg/g. To simulate a worst-case scenario, the PM emission yield input for the model was calculated by taking the average value plus the positive standard deviation, which produced a yield of 52 mg/g of cell mass for NMC cells. It was noted that this yield is similar to the 0.05 kg/kg (50 mg/g) utilized by Franqueville et al. (2023) [47]. The weight of each cell in the modeled BESS unit was assumed to be 2.99 kg. As such, the total mass of the 6,384 cells in the modeled unit was 19,088 kg and the total mass of the 1,008 cells in one bay of the modeled unit was 3,014 kg. Therefore, it was estimated that a total of 993 kg of particulate matter would be produced over the duration of an event involving the entire unit, which is representative of the flaming scenario. A total of 157 kg of particulate matter will be produced over the duration of an event involving one bay, which is representative of the non-flaming scenario.

NOTE FOR USERS

The total mass of particulates produced calculated here is specific to the size/mass of the BESS unit that was modeled. When evaluating specific BESS units, the user must utilize specifications for the equipment being considered.

For LFP cells, Wang et al. (2023) found that the particulate yield, for particle sizes less than 900 μm , was 55 mg/g of fuel. However, as in Zhang et al. (2019a) and (2019b), the particle quantification did not include particles which did not settle (i.e., PM_{2.9}) [85]. Therefore, to conservatively account for the particles not quantified in the settleable PM, a 1% increase was applied to the PM emissions factor. Utilizing this methodology, the PM emission yield is 56 mg/g. It was noted that this yield is similar to the yield for the NMC cells (52 mg/g). For the modeled BESS unit, using this yield, it was estimated that a total of 1,069 kg of particulate matter would be produced over the duration of an event involving the entire unit, which is representative of the flaming scenario. A total of 169 kg of particulate matter was estimated to be produced over the duration of an event involving one bay, which is representative of the non-flaming scenario.

Essl et al. (2020a) also looked at particle production for NMC cells under non-flaming conditions, however, the analysis methods used in the study do not allow for reasonable extraction of data for the model. Particle sampling was performed via an air stream, therefore, only data for smaller size particles was provided (11 μm or smaller). In addition, the total mass of particles produced was not directly determined [64] and the reported particle yields of 807 mg/g of mass lost, and 347 mg/g of the starting cell mass, are expected to be artificially high due to lack of consideration for condensed gases, liquids, and large pieces of ejected cell contents.

For flaming conditions, the literature review did not reveal any studies that were determined to provide usable particulate matter yields. INERIS (2022) reported a soot yield value of 2.1 g/g for NMC cells at 50% SOC [87], however, the magnitude of this value does not make sense, as the mass produced in soot cannot be greater than the starting mass. No additional information was provided on the samples tested, test configuration, measurement techniques, or composition of the soot [87]. As such, the integrity of this data point could not be evaluated and therefore, was not used. Premnath et. al. (2022) looked at airborne PM_{2.5} and smaller but did not report total quantities or mass yields. Additionally, they did not capture the production of larger, settleable particles [88] and, therefore, the data was not utilized in the model inputs. Due to the lack of data for flaming conditions, the particulate yields for NMC and LFP cells established for the non-flaming scenarios were also utilized in the flaming scenarios.

4.4.2. Particulate Size Distribution

Three studies assessed particle size distribution for NMC cells [81][84][86]. These three studies were performed by the same authors in the same lab group. Zhang et al. (2019a) found that of the settleable PM, 44% were 2.9 μm to 850 μm in diameter. Of this PM size group, 90% was 457 μm or less, 50% was 198 μm or less, and 10% was 22.5 μm or less [81]. Zhang et al. (2019b) found that of the settleable PM, 90% was 500 μm or less. Of this PM size group, 90% was 390 μm or less, 50% was 195 μm or less, and 10% was 19 μm or less [86]. Wang et al. (2020) conducted a similar experiment with a focus on PM₅₀₀. The authors reported a size distribution by mass of 0.005% at 30 μm or less, 8.48% at 30 to 50 μm , 41.3% at 50 to 100 μm , 34.5% at 100 to 250 μm , and 15.8% at 250 to 500 μm [84]. The data from these three studies was grouped into particle size

ranges that overlapped as much as possible, at the discretion of the authors. The average percent mass of PM in each group was calculated. Table 20 provides the particle size distribution utilized for the NMC cell chemistry scenarios. Only data for non-flaming conditions was found, therefore the same particle size distribution was used in both non-flaming and flaming model scenarios.

Table 20. NMC particulate size distribution.

Mass % of Particulates by Particle Diameter [μm] for NMC Cells					
$d \leq 20$	$20 < d \leq 50$	$50 < d \leq 150$	$150 < d \leq 300$	$300 < d \leq 500$	$500 < d \leq 850$
4%	9%	31%	35%	14%	7%

One study assessed particle size distribution for LFP cells. This study found that of the settleable PM, 55% was 3000 μm or less in diameter and 26% was 300 to 900 μm. Of the raw, non-agglomerated particles, 90% was 349 μm or less, 50% was 141 μm or less, and 10% was 13 μm or less [85]. Table 21 provides the particle size distributions utilized for the LFP cell chemistry scenarios. Only data for non-flaming conditions was found, therefore the same particle size distribution was used in both non-flaming and flaming model scenarios.

Table 21. LFP particulate size distribution.

Mass % of Particulates by Particle Diameter [μm] for LFP Cells			
$d \leq 13$	$13 < d \leq 141$	$141 < d \leq 349$	$349 < d \leq 900$
10%	40%	40%	10%

NOTE FOR USERS

The particulate size distribution groupings established here were determined based on the available experimental data. AERMOD does not require specific groupings for particulate size distribution. Therefore, if other data is utilized, the groupings can be revised to provide the best fit.

4.4.3. Particulate Composition

Appendix 7.1 presents the findings from the literature review on the metal composition of particulates from flaming and non-flaming thermal runaway in NMC cells. It is noted that the mass composition percentages from Bordes et al. (2022) did not consider organic particles (e.g. carbon) [63]. Therefore, to be utilized, these values needed to be adjusted to a percent of total PM. Zhang et al. (2019a) reported that for PM₈₅₀, 30.1% was carbon [81], and Zhang et al. (2019b) found that 28% was carbon and 12.3% was oxygen [86]. Taking the data from these two studies, the average inorganic PM content was approximately 65%. Therefore, to obtain an estimated mass composition of metals in the total PM for the data from Bordes et al. (2022), values were adjusted to be 65% of the reported values. Table 22 presents the average values from the data in Appendix 7.1, with adjustments for Bordes et al. (2022) [63], which were used in the model. While metallic elements were identified aside from lithium, nickel, manganese, and cobalt, only copper and aluminum accounted for a significant portion (>1% mass). Other metals were 2 to 4 magnitudes smaller and were not included in the model.

Table 22. Particulate composition for NMC cell chemistry.

Condition	Particulate Composition [% Mass]					
	Li	Ni	Co	Mn	Al	Cu
Non-Flaming	3.5	25.0	9.3	8.0	6.3	5.4
Flaming	3.7	19.5	16.0	14.5	3.9	0.0

Data on LFP particulate composition was not found. However, the metallic cell composition of an LFP cell is expected to be like other Li-ion cells except for the anode and cathode chemistry. Thus, the composition of the NMC cells as shown in Table 22 was taken as a base model. It was assumed that nickel, manganese, and cobalt would not be present in the particulate matter since they are unique to NMC cell chemistry. Therefore, the mass percentages were adjusted assuming that lithium and iron would each increase by 30% of the mass attributed to nickel, manganese, and cobalt in NMC cells. All other elements (aluminum and copper) were assumed to be present at equivalent amounts. Table 23 provides the final particulate composition inputs for modeling of LFP cell scenarios.

Table 23. Particulate composition for LFP cell chemistry.

Condition	Particulate Composition [% Mass]			
	Li	Al	Cu	Fe
Non-Flaming	17.5	6.3	5.4	14.4
Flaming	20.4	3.9	0	16.6

It was assumed that particulate composition is homogeneous for all particulate matter, i.e., the composition does not change by sample.

4.5. Meteorological Conditions

4.5.1. Fire Dynamics Simulator

The FDS modeling included a sensitivity analysis for wind and temperature using minimum, average, and maximum conditions. The plume was modeled over a relatively flat terrain. Weather conditions were chosen based on southern California, as it is one of the areas in the U.S. where BESS installations are prevalent. The meteorological parameters for FDS are presented in Table 24.

Table 24. FDS model weather inputs.

	Minimum	Average	Maximum
Wind [m/s (mph)]	2 (4.47)	5 (11.18)	10 (22.37)
Temperature [°C (°F)]	7 (45)	22 (72)	35 (95)

Note: Adapted from Weather Spark. Climate and Average Weather Year-Round in California [89].

The Monin-Obukhov Similarity was applied in FDS to account for the change in wind velocity by height due to the boundary layer. FDS requires inputs for base windspeed, which is provided in Table 24, reference height, terrain roughness, thermal stability, and temperature lapse rate. The reference height chosen was 10 m since weather stations in the U.S. typically read surface wind measurements at this height. A roughly open terrain ($z_0 = 0.1$) was chosen to mimic the base conditions (flat terrain with low-lying vegetation). The model was run with a very thermally unstable parameter ($L = -100$ m). Temperature lapse rate was set to 0°C/m , which created a constant temperature profile with height.

NOTE FOR USERS

The terrain characteristics, wind conditions, ambient temperatures, temperature lapse rate, and atmospheric stability can all be site-specific parameters. The user should assess the location at which the BESS unit is located and apply the relevant meteorological and geographical data.

4.5.2. AERMOD

Unlike FDS and Pyrosim, AERMOD utilizes meteorological inputs from real-world weather readings processed through AERMET. The AERMET meteorological file provides information on hourly variations in surface wind and direction, ambient temperature, boundary layers, relative humidity, pressure, precipitation, and cloud cover. The weather station selected was Lemoore Airport, California as it is surrounded by flat terrain with low-lying vegetation, which mimics the FDS simulation topography. The most recent weather readings available for Lemoore were from 2022. Since wind speeds and temperatures vary by the hour, it was difficult to find specific times where the wind speed and temperature would match the inputs for the FDS/Pyrosim simulations. Additionally, factors aside from wind speed and temperature provided in the AERMET file would change the plume dispersion behavior. Given that the weather readings were too inconsistent for comparison, a sensitivity analysis was not performed for wind and temperature in AERMOD. Instead, the data from June 22, 2022, was chosen as a baseline for evaluation as it had readings close to the highest wind speed and temperature modeled in FDS (10 m/s and 35°C), as well as readings close to 22°C and the other wind speeds (2 and 5 m/s). Simulations were run for the full duration of the day. Concentrations were calculated by averaging values over the defined scenario durations, e.g. 0.5-, 1-, 2-, 4-, and 6-hour periods, such that AERMOD could plot the change in concentration throughout the day. There was no precipitation on June 22, 2022. All AERMOD simulations were run within this day, with outputs consisting only of maximum 1-hour average concentration values from the day. As such, the impact of varying wind and temperature conditions could not be assessed.

NOTE FOR USERS

For a site-specific analysis, the location selected in AERMOD should represent the actual project location. To evaluate a range of meteorological conditions that could be expected, it may be necessary to perform simulations for multiple days throughout the year.

4.6. *AERMOD View Point Source Inputs*

The point source method requires inputs for emission rate in g/s, gas exit temperature in K, stack inside diameter in m, gas exit velocity in m/s or gas exit flow rate in m³/s, and release height in m. If the user inputs gas exit velocity, gas exit flow rate is calculated and vice versa.

For the non-flaming scenarios, the gas venting temperature calculated in Section 4.2.1 and the total gas production rate calculated in Section 4.2.1 were used as the gas exit temperature and flow rate, respectively. However, the same data was not readily available for the flaming scenarios, as these are influenced by the combustion conditions. Instead, plume temperature and velocity were extrapolated from the FDS data. This was achieved by applying y-axis 2D slices in the Pyrosim model at the approximate centerline of the plume and z-axis 2D slices at the approximate height at which combustion within the plume ceased. The FDS simulation data was processed using pyFDSools, a Python package developed by Hodges (2020) that assists in developing and post-processing FDS data. The Python package generates plots and Excel sheets from the 2D-slice files in FDS [90].

Velocity and temperature were averaged for each constituent over the period at which the plume had reached steady state to generate an excel sheet of the 2D slice. The y-axis 2D slice data was used to identify the plume centerline velocity at the z-axis 2D slice height. The plume boundaries were then determined based on points at which the gas velocity had declined to one-half the centerline velocity, in accordance with methodologies presented by Heskestad (2016) [91]. This revealed that the plume had an elliptical shape, which was congruent with the visual results of the FDS model. The approximate area of the ellipse was used to determine the stack diameter for AERMOD. The average temperature and velocities of the plume within the defined boundaries were calculated and used as the gas exit temperature and velocity in AERMOD. Due to potential impacts of wind, gases were set to release at 2.5 m, the height of the BESS unit, which is a more conservative approach than utilizing the heights at which the plume temperatures and velocities were determined. Table 25 shows the gas exit temperature⁷, velocity, and flow rate inputs for each modeled scenario.

Table 25. AERMOD View point source inputs.

Thermal Runaway Conditions	Cell Chemistry	Gas Exit Temperature ¹ [K]	Gas Exit Velocity [m/s]	Gas Exit Flow Rate [m ³ /s]
Non-flaming	LFP	505	-	0.0125
	NMC	602	-	0.207
Flaming	LFP	499	8.5	-
	NMC	409	5.9	-

⁷ Table 53 shows that the gas exit temperature input utilized in the flaming scenario is lower than the non-flaming scenario. This is due to the methodology used to capture the characteristics of the plume at a point above the combustion reaction. With this methodology, the values indicated for the flaming scenario represent the average temperature of gases released from the BESS unit combined with the ambient air that has been entrained into the plume.

4.7. *Methods to Evaluate Health Impact*

There are various human health exposure guidelines in the United States that have been developed, primarily, by the National Institute for Occupational Safety and Health (NIOSH) [92], the American Conference of Governmental Industrial Hygienists (ACGIH) [93], the EPA [94], and the U.S. Department of Energy (DOE) [95]. The various exposure limits defined by the aforementioned organizations are widely used and accepted in the safety and health industry, and in some cases, are mandated through statutes. Plume gas concentrations in the models were compared to these exposure guidelines to determine the furthest distance at which concentrations exceeded guideline thresholds within the computational domain.

Health impact was analyzed using the outputs from FDS/Pyrosim in the near-field (up to 200 m) and AERMOD View in the far-field (up to 2.5 km). Gas concentrations were evaluated at 1.5 m, the breathing height of the average human. In the Pyrosim/FDS model, 2D-slice files were added at breathing height to record concentrations during the simulation. pyFDSools was utilized to generate excel sheets and concentration plots for the gas concentrations. Concentrations were averaged for each constituent over the period at which the plume had reached the end of the domain and become steady. Exposure limit distances were evaluated by finding the furthest point downwind, or to the side, of the BESS unit where concentrations exceeded either occupational (IDLH) or community (AEGL-1, ERPG-1, or TEEL-1) exposure limits within the domain. If a gas was above an exposure limit at the furthest points in the FDS domain, it was documented in the results but not evaluated outside of the boundaries of the domain. Simulations varied by cell chemistry, thermal runaway conditions, wind speed, temperature, and incident duration. A total of 108 simulations were run using FDS/Pyrosim to evaluate near-field health impact.

Since AERMOD View was primarily utilized for far-field dispersion, only community exposure guidelines were evaluated in simulations run in AERMOD. Gas concentrations were averaged throughout the day and plotted using the contour function. An averaging period of 1 hour was chosen because the Protective Action Criteria (PACs) hierarchy calculates exposure limit guidelines based on 1-hour exposure durations [96]. The contour function provides a concentration plot of the maximum concentration values found when averaging over the 1-hour periods throughout the day. Concentrations were converted from $\mu\text{g}/\text{m}^3$ to ppm and evaluated at community exposure guidelines. Exposure limit distances were evaluated by finding the furthest point downwind where concentrations exceeded community exposure limits during the day. Simulations varied by cell chemistry and thermal runaway conditions. For the flaming scenarios, the average incident duration (4 hours) was selected for modeling. For the non-flaming scenarios, there was not an average incident duration. Instead, the minimum incident duration was selected for modeling as it would produce plume constituents at a higher rate. The minimum incident duration for the LFP non-flaming scenario was 6 hours. The minimum incident duration for the NMC non-flaming scenario was 0.5 hours. A total of 9 simulations were run using AERMOD View to evaluate far-field health impact.

4.7.1. Occupational Exposure

Occupational exposure levels were assessed to focus on the impact on those in the immediate vicinity of the equipment, e.g., emergency response personnel. The IDLH values were developed by NIOSH to protect workers from high-risk exposures to toxic chemicals in the workplace and to determine when (and what type of) respiratory protection is required. The IDLH values represent

the maximum airborne concentrations a healthy adult worker (without a respirator) could be exposed to for 30 minutes without suffering permanent or escape-impairing health effects [92].

Table 26 presents the IDLH values for the evaluated toxic gases.

Table 26. IDLH Guidelines.

Chemical	IDLH [ppm]
Benzene	500
CO	1200
CO ₂	40,000
HF	30
HCl	50
HCN	50
HBr	30
NO ₂	13
SO ₂	100

Note: Adapted from NIOSH, Immediately Dangerous To Life or Health (IDLH) Values, February 2021 [97].

The steady state gas concentrations of all constituents were evaluated at IDLH to determine if a negative health impact is likely based on distance from the enclosure and weather conditions. Concentrations were evaluated downwind of and in the area surrounding the BESS unit. Justifications for IDLH values from NIOSH are provided in Appendix 7.3.

4.7.2. Community Exposure

In this study, it was assumed that the public and communities were not in the immediate vicinity of the BESS unit. As such, acute exposure guidelines, rather than IDLH limits, were used to evaluate community health impact and to aid in determining recommendations for shelter-in-place or evacuation.

The PACs is a database provided by the DOE that compiles emergency exposure limits for uncontrolled release of hazardous chemicals. These values are used to evaluate the severity of the event and provide the necessary information to plan emergency response. The PACs hierarchy requires that final and interim 1-hour exposure duration Acute Exposure Guideline Levels (AEGL) values are used preferentially, followed by Emergency Response Planning Guidelines (ERPG) values, then Temporary Emergency Exposure Guidelines (TEEL) values when evaluating consequences [96]. The EPA AEGL are used for rare releases of chemicals into the air, such as the toxic gas production that occurs during an unwanted fire event. The AEGLs are provided for a range of exposure doses at which the general population and susceptible individuals will experience a given impact. There are three levels of AEGL guidelines associated with different health effects and are defined by the EPA as follows:

1. **AEGL-1:** “The concentration of a substance above “which it is predicted that the general population could experience, including susceptible individuals, notable discomfort, irritation, or certain asymptomatic non-sensory effects.”
2. **AEGL-2:** “The concentration of a substance above which it is predicted that the general population could experience, including susceptible individuals, could experience

irreversible or other serious, long-lasting, adverse health effects or an impaired ability to escape.”

3. **AEGL-3:** “The concentration of a substance above which it is predicted that the general population could experience, including susceptible individuals, life-threatening health effects or death.” [94]

Each AEGL is divided into exposure for 10 minutes, 30 minutes, 1 hour, 4, hours, and 8 hours [94]. Depending on the chemical, the AEGL may change due to the dose-time relationship. For the purposes of this study, exposure considerations will be limited to AEGL-1 as evacuation or shelter-in-place orders would need to be given before irreversible health effects or impairment of ability to escape. Table 27 provides a list of AEGL-1 values for the evaluated toxic gases.

Table 27. AEGL-1 (1-hour) Guidelines.

Chemical	1-hour Exposure Duration AEGL-1 [ppm]
Benzene	52
CO	See Note a.
CO ₂	See Note b.
NO	See Note a.
NO ₂	0.50
HF	1.0
HCl	1.8
HCN	2.0
HBr	1.0
SO ₂	0.20

a. Data is insufficient, no guideline established.

b. Not assessed.

Note: Adapted from EPA, Access Acute Exposure Guideline Levels (AEGLs) Values, retrieved 10/22/2024 [98].

Justifications for AEGL-1 values from the EPA are provided in Appendix 7.4.

The ERPGs were developed by the American Industrial Hygiene Association (AIHA). Unlike AEGLs, ERPGs are not designed with susceptible individuals in mind. The ERPGs are also divided into three tiers based on different health effects. These tiers are defined by the AIHA as follows:

1. **ERPG-1:** “The maximum airborne concentration below which nearly all individuals could be exposed for up to 1 hour without experiencing more than mild, transient adverse health effects or without perceiving a clearly defined objectionable odor.”
2. **ERPG-2:** “The maximum airborne concentration below which nearly all individuals could be exposed for up to 1 hour without experiencing or developing irreversible or other serious health effects or symptoms which could impair an individual's ability to take protective action.”
3. **ERPG-3:** “The maximum airborne concentration below which nearly all individuals could be exposed for up to 1 hour without experiencing or developing life-threatening health effects” [93].

Similarly, for the purposes of this study, exposure considerations will be limited to ERPG-1. Table 28 provides a list of ERPG-1 values for the evaluated toxic gases.

Table 28. ERPG-1 Guidelines.

Chemical	ERPG-1 [ppm]
Benzene	See Note a.
CO	200
CO ₂	See Note b.
NO	See Note b.
NO ₂	See Note a.
HF	See Note a.
HCl	See Note a.
HCN	See Note a.
HBr	See Note a.
SO ₂	See Note a.

a. AEGL values were available, therefore ERPG values were not provided

b. Not assessed.

Note: Adapted from NOAA, CAMEO Chemicals, retrieved 10/22/2024 [99].

The TEELs were developed by the DOE and are used to evaluate short-term chemical releases when neither AEGLs nor ERPGs are available. TEELs are designed with both the general population and susceptible individuals in mind. Unlike AEGLs and ERPGs, TEELs are not derived from review of animal and human studies. Recognizing that the method of defining AEGLs and ERPGs is more accurate, TEELs are replaced when an AEGL or ERPG value is available. The TEELs are also divided into three tiers based on different health effects. These tiers are defined by the DOE as follows:

1. **TEEL-1:** “The airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, when exposed for more than one hour, could experience notable discomfort, irritation, or certain asymptomatic, nonsensory effects. However, these effects are not disabling and are transient and reversible upon cessation of exposure.”
2. **TEEL-2:** “The airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, when exposed for more than one hour, could experience irreversible or other serious, long-lasting, adverse health effects or an impaired ability to escape.”
3. **TEEL-3:** “The airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, when exposed for more than one hour, could experience life-threatening adverse health effects or death.” [95]

Similarly, for the purposes of this study, exposure considerations will be limited to TEEL-1.

Table 29 provides a list of TEEL-1 values for the evaluated toxic gases.

Table 29. TEEL-1 Guidelines.

Chemical	TEEL-1 [ppm]
Benzene	See Note a.
CO	See Note a.
CO ₂	30,000
NO	0.5
NO ₂	See Note a.
HF	See Note a.
HCl	See Note a.
HCN	See Note a.
HBr	See Note a.
SO ₂	See Note a.

a. AEGL and ERPG values are available, therefore TEELs were not provided.

Note: Adapted from NOAA, CAMEO Chemicals, retrieved 10/22/2024 [99].

The steady state gas concentrations derived from the non-flaming and flaming models were compared against the 1-hour AEGL-1, ERPG-1, and TEEL-1 values to determine if a negative health impact is likely based on distance from the enclosure and weather conditions. AEGL-1, ERPG-1, and TEEL-1 values were utilized to evaluate only the area downwind of the BESS unit within the domain. Further, it was assumed the public and communities are not in the immediate vicinity of the BESS unit.

4.8. *Methods to Evaluate Environmental Impact*

The environmental impact of BESS thermal runaway is heavily dependent on the surrounding area. Topography, precipitation, soil type, bodies of water, and the flora and fauna living in the surrounding area vary significantly by region. Furthermore, the mode of pollution, i.e., firewater runoff or deposition, will also affect the degree of impact. As such, a general method for assessing environmental impact is provided within this study.

NOTE FOR USERS

To apply this method to a specific case, it is necessary that the user identify the unique characteristics of the possible areas of impact and adjust their scenario accordingly.

4.8.1. *Impacts via Deposition*

The study focused on the impact on the environment through deposition of soot particulate falling out of the plume. In this scenario, particulate can deposit onto either the surface soil or surface water. For acute exposure, it is expected that contamination will not have reached groundwater yet. The environmental impact on air was not evaluated in this study as no relevant guidelines were found. The Ecological Structure Activity Relationships (ECOSAR) Database, established and maintained by the EPA for approximately 30 years, does not provide guidelines

for air [100]. The European Chemicals Agency (ECHA) provides Predicted No-Effect Concentration (PNEC) values for air for various chemicals; however, air impact was designated as not applicable by ECHA for the identified metal constituents [101]. Other air pollution guidelines, such as AQI, relate chemical releases back to human health and, therefore, would not be appropriate for evaluation of environmental impact.

Environmental impact was analyzed using the particle deposition function in AERMOD View. The location of the modeled BESS unit was set to Lemoore, CA. The area is rural and located in a land-locked valley with bodies of freshwater. It was assumed that there are no other sources of pollution aside from the BESS unit thermal runaway event and the background concentrations of all metals are 0. The terrain was set to flat under rangeland use to mimic a location with flat, low-lying vegetation and no surrounding buildings. No background emissions or downwash from buildings were included in the model. Deposition was evaluated at 0 m under the assumption that the terrain is flat. Simulations varied by cell chemistry and thermal runaway conditions. For the flaming scenarios, the average incident duration (4 hours) was selected for modeling. For the non-flaming scenarios, there was not an average incident duration. Instead, the minimum incident duration was selected for modeling as it would produce plume constituents at a higher rate. The minimum incident duration for the LFP non-flaming scenario was 6 hours. The minimum incident duration for the NMC non-flaming scenario was 0.5 hours.

NOTE FOR USERS

The terrain characteristics and surrounding built environment are site-specific parameters. The user should assess the location at which the BESS unit is located and apply the relevant geographical data.

The total surface deposition was calculated for the entire incident duration (30-minute, 4-, or 6-hour period) throughout the day and plotted using the contour function. The total incident duration was utilized as the deposition would accumulate throughout the incident. A full analysis of one scenario was performed as an example of the environmental impact assessment methodology. The NMC flaming scenario was chosen for analysis as it produced the highest concentrations of PM deposition furthest away from the BESS unit. Deposition within the computational domain was found and compared to environmental exposure guidelines.

There are several guidelines for evaluating environmental impact via water and soil. The EPA provides values for Lethal Concentration 50 (LC₅₀) and Effective Concentration 50 (EC₅₀) to define acute (short-term) toxicity in the environment in ECOSAR. While ECOSAR is primarily utilized for aquatic environments, it also provides toxicity values for terrestrial environments where data is available. ECOSAR is not validated for predicting toxicity for chemicals with a molecular weight over 1,000 g/mol [102]; however, that does not apply to the metals of interest in this study. LC₅₀ is the concentration at which 50% of the animals exposed to an acute dose are expected to die and can be obtained from acute toxicity studies assessing pollution. EC₅₀ is the concentration where there is either a 50% reduction in growth, growth rate, or immobilization. LC₅₀ and EC₅₀ values were utilized in this study, because they are more readily available and are derived from species-specific testing. Other values like PNEC or No Observed Effect Level (NOEL) are typically derived, i.e., calculated, from the LC₅₀ and EC₅₀ test data [103]. If a more conservative approach is desired, the relevant stakeholder or user can use PNEC or NOEL values, where such data exists for the constituent(s) of interest.

LC₅₀ and EC₅₀ values for each metal effluent were gathered utilizing ECOSAR [100]. The EPA provides LC₅₀ and EC₅₀ for fish, *daphnia magna*, algae, and mysids for aquatic toxicity. Comprehensive data sets exist for freshwater fish with limited data on saltwater fish. According to the EPA, the ECOSAR program focuses on freshwater fish “because most releases of industrial chemicals go to freshwater bodies.” As such, only the values for freshwater fish were provided in Table 30. The LC₅₀ values are derived from a 96-hour exposure duration for fish and mysids. The EC₅₀ values for *daphnia magna* are reported for 48-hour exposures, and EC₅₀ values for algae are reported for 96-hour exposures. LC₅₀ values for earthworms under a 14-day exposure duration are also provided by ECOSAR for quantification of soil toxicity (ECOSAR) [102]. All these durations are considered short-term exposure periods but exceed the typical duration of a BESS event and thus are conservative.

As an additional conservative measure, the initial water and soil concentrations produced from the BESS thermal runaway incident were assumed to remain in the substrate with no dilution, leaching, runoff, etc. Table 30 lists the LC₅₀ and EC₅₀ values for common metal emissions from Li-ion battery thermal runaway.

Table 30. LC₅₀ and EC₅₀ values.

Species	LC ₅₀ [mg/L]			EC ₅₀ [mg/L]	
	Freshwater fish	Mysid	Earthworm	<i>Daphnia Magna</i>	Algae
Li	1760	10600	23.4	772	200
Ni	9280	51600	189	4400	1230
Mn	1760 ^a	5400 ^a	146 ^a	848 ^a	321 ^a
Co	1890	5790	156	909	344
Al	781 ^a	2240 ^a	77.7 ^a	380 ^a	150 ^a
Cu	10600	55900	204	4760	1330

a. No effect at saturation.

All four aquatic organisms (fish, mysid, *daphnia magna*, algae) identified in Table 30 are commonly found in freshwater areas. Thus, it was expected that they would be present in a water source in a land-locked area such as Lemoore, CA. The most sensitive species is the green algae, so its EC₅₀ values were chosen as the environmental assessment endpoint.

NOTE FOR USERS

An environmental assessment includes an analysis of the surrounding animals to determine which species-specific values are applicable. Then, the most conservative value can be chosen as the guideline for determining environmental impact.

AERMOD provides surface deposition concentration in g/m². Surface deposition was converted to mg/L using a reference depth. It is assumed that soil deposition would be primarily confined to the surface soil immediately following the incident. The International Atomic Energy Agency (IAEA) defines surface soil as the first 0 to 3 in (0 to 0.076 m) from the surface [104]. Earthworms typically live within the top 15 to 20 in (0.38 to 0.51 m) of soil [105], so the surface

soil region would be applicable for the earthworm EC₅₀ values. For the purposes of this study, the reference depth was 0.076 m for soil contamination.

The EPA recommends that samples are collected in areas downstream of turbulence such that the water is well mixed (EPA, 1996). Assuming that the body of water is well-mixed, and the metal concentrations are consistent throughout, the applicable reference depth would be the depth of the body of water. Mixing is more likely to occur in a river or a stream compared to sluggish or a standing body of water such as a lake, so the relevant stakeholder or user would need to determine the appropriate reference depth where depth profiling is relevant [106]. The closest major body of water to Lemoore is the Kings River, approximately 7 to 8 km away. To assess potential impacts on bodies of water that may be closer, this distance was assumed to be 1 km in this study. Gauge height data for Kings River near Lemoore is recorded by the U.S. Geological Survey [107]. Data for June 22, 2022, is not available; however, there is data for 2023 to 2024. On June 22, 2023, gauge height was approximately 16.4 ft (5.00 m). On June 22, 2024, gauge height was approximately 15.4 ft (4.69 m) [107]. The average gauge height, 15.9 ft (4.85 m), was used as the reference depth for the purposes of this study.

NOTE FOR USERS

The bodies of water that may be impacted by particulate deposition will be site-specific. In an environmental impact assessment for a specific project, these bodies of water should be identified along with their distance from the project site and characteristic depths. Due to wind direction or remote plume grounding, the closest body of water may not always be the most impacted.

4.8.2. Impacts via Water Runoff

Aside from combustion products, contaminated water runoff due to firefighting operations (fire water runoff) can carry toxic compounds. Fire water runoff can enter the soil, groundwater, or nearby bodies of water, thus contaminating the environment. Humans may encounter toxic compounds that were absorbed into the environment or ingest toxic compounds that become built up in food products [108]. Contaminated water via rainfall is also possible; however, because the quantity of water that will come into contact with the burning/burned materials is expected to be orders of magnitude less, this is less of a concern than environmental impacts caused by fire water runoff.

The environmental impact of contaminated water runoff from a fire is dependent on several factors including the contaminant, the starting concentration of the contaminant in the water, the path on which the water travels (e.g., soil, waterways, hard surfaces), the final destination of the water (e.g., farmland, lake, ocean), and the exposed subject (e.g., plant, animal). As such, what happens to the contaminant in the water after it leaves the fire location and the impact it makes is extremely dependent on the surrounding topography and geographical conditions, to an even greater degree than airborne contaminants. It was outside of the scope of this study to provide a specific hazard analysis related to fire water runoff. The scope of evaluation on fire water runoff was limited to the starting concentration of contaminants at the fire source location.

The literature review revealed several studies [109][110][111][76] that examined contamination of fire water. Table 31 summarizes the concentrations of elements and chemicals that were found to be elevated in these studies. For each study, the quantity of water, normalized by energy capacity of the Li-ion battery/module used in the test are indicated.

Table 31. Concentrations of Chemicals found in firewater runoff from various studies of Li-ion thermal runaway events.

	Bordes (2024) [109] [mg/L]			Held (2022) [110] [mg/L]		Long (2013) [111] [mg/L]		Quant (2023) [76] [mg/L]
Al	74.2	29.3	73.9	-	-	3	1	4
Ba	-	-	-	-	-	0.6	0.3	-
Co	0.42	12.8	7.07	36	50	0.02	0.8	0.02
Cr	-	-	-	-	-	-	-	0.001
Cu	0.30	0.26	4.18	-	-	0.2	0.1	0.01
Fe	5.92	4.59	0.30	-	-	0.7	0.2	-
Li	44.5	27.8	360	7	1,460	0.3	3.6	71
Mn	1.22	17.0	5.82	36	53	0.3	4.6	0.11
Mo	-	-	-	-	-	-	-	0.07
Ni	3.25	49.0	40.1	36	55	0.1	0.7	0.05
Sb	-	-	-	-	-	0.7	0.7	0.01
Zn	-	-	-	-	-	29	2.7	-
16-PAH	0.004	0.013	0.009	0.0019	0.00011	-	-	<DL
EMC	138	59	-	-	-	-	-	-
EC	1082	461	-	-	-	-	-	-
Chloride	33.4	36.5	203	2	22	143	60	43
Fluoride	142	91.6	93.7	8	330	27	33	57
Quantity of Water Applied in Test (L/Wh)	0.014	0.024	0.01	0.07	0.012	0.91	0.28	0.22

DL= Detection Limit

The results of these studies were compared to the same regulatory thresholds outlined in Section 4.8.2 for the identified contaminants. This high-level analysis was used to identify the potential of an outdoor BESS thermal runaway incident to negatively impact plants and animals via contaminated fire water runoff. This evaluation was limited to the BESS unit that experienced thermal runaway, not adjacent units to which water may be applied to prevent ignition.

5. Results and Discussion

The results in this section represent a range of possible gas concentration profiles and exposure limit distances that could result from different types of BESS thermal runaway events. The results are derived from the full range of HRR, THR, MLR, and gas species data currently available in the literature for NMC and LFP chemistries. The results are not intended to represent outcomes of a thermal runaway event in a specific product and should not be used in that manner without verifying that the inputs are applicable to the product and likely failure scenario(s). The analysis using FDS/Pyrosim focused on health impact in the near-field (up to 200 m), whereas the analysis using AERMOD View focused on health impact and environmental impact in the far-field (up to 2.5 km).

5.1. Fire Dynamics Simulator

Figure 6 through Figure 9 show the MLR and species gas production rates from FDS/Pyrosim for each cell chemistry and thermal runaway condition (non-flaming vs. flaming) for the shortest incident duration. For the LFP and NMC non-flaming scenarios, the shortest incident duration was 6 and 0.5 hours, respectively. For the flaming scenarios, the shortest incident duration was 2 hours. The MLR and species gas production rate curves for longer incident durations have the same trends as the graphs presented below. Graphs for the species gas production rates were separated for clarity. For the flaming scenarios, CO and CO₂ are not shown in the graphs as they were factored into the yields produced by the combustion reaction. As such, FDS does not provide the MLR by species for these gases.

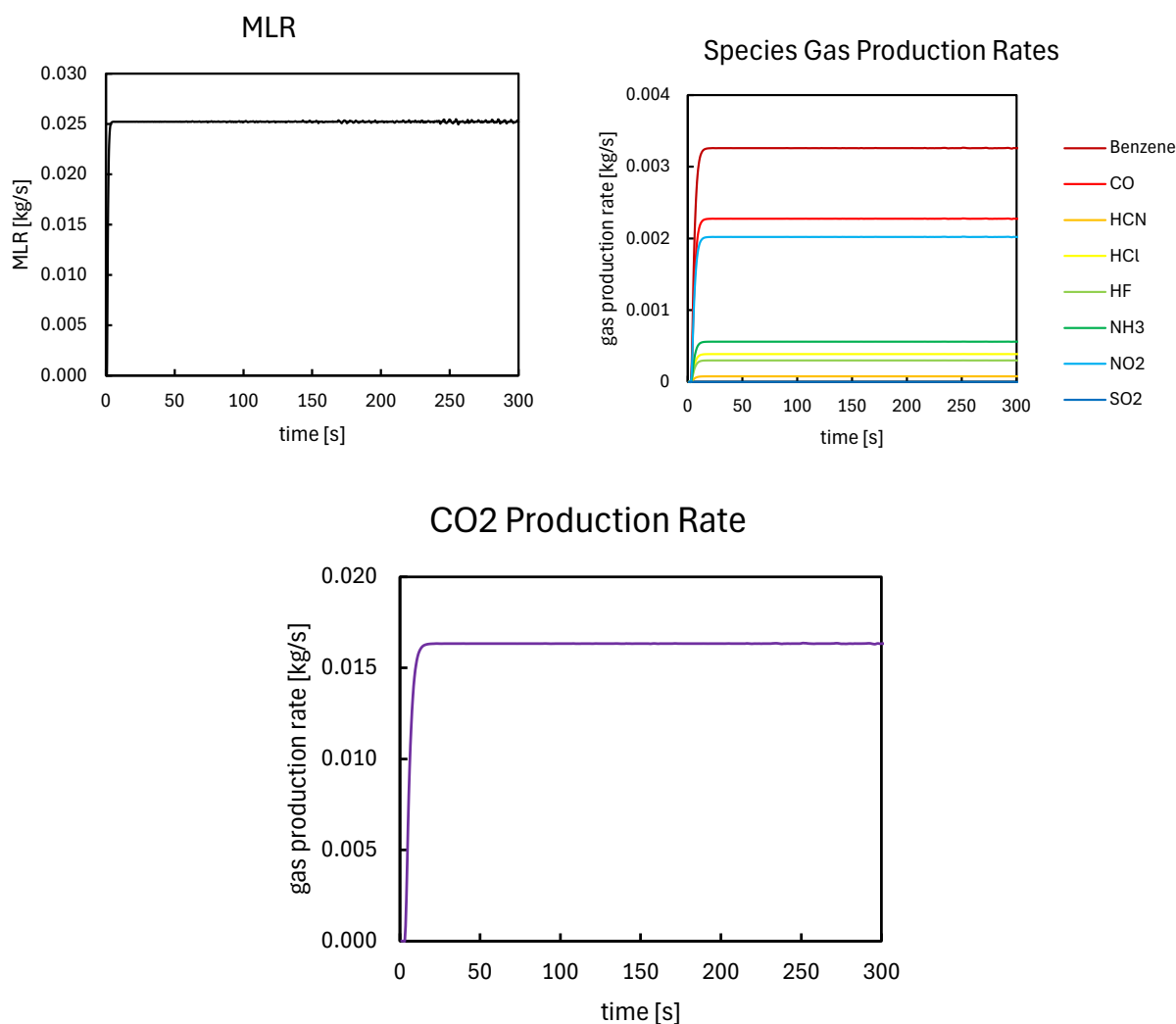


Figure 6. MLR and species gas production rates from FDS/Pyrosim for the LFP non-flaming scenario at a 6-hour incident duration.

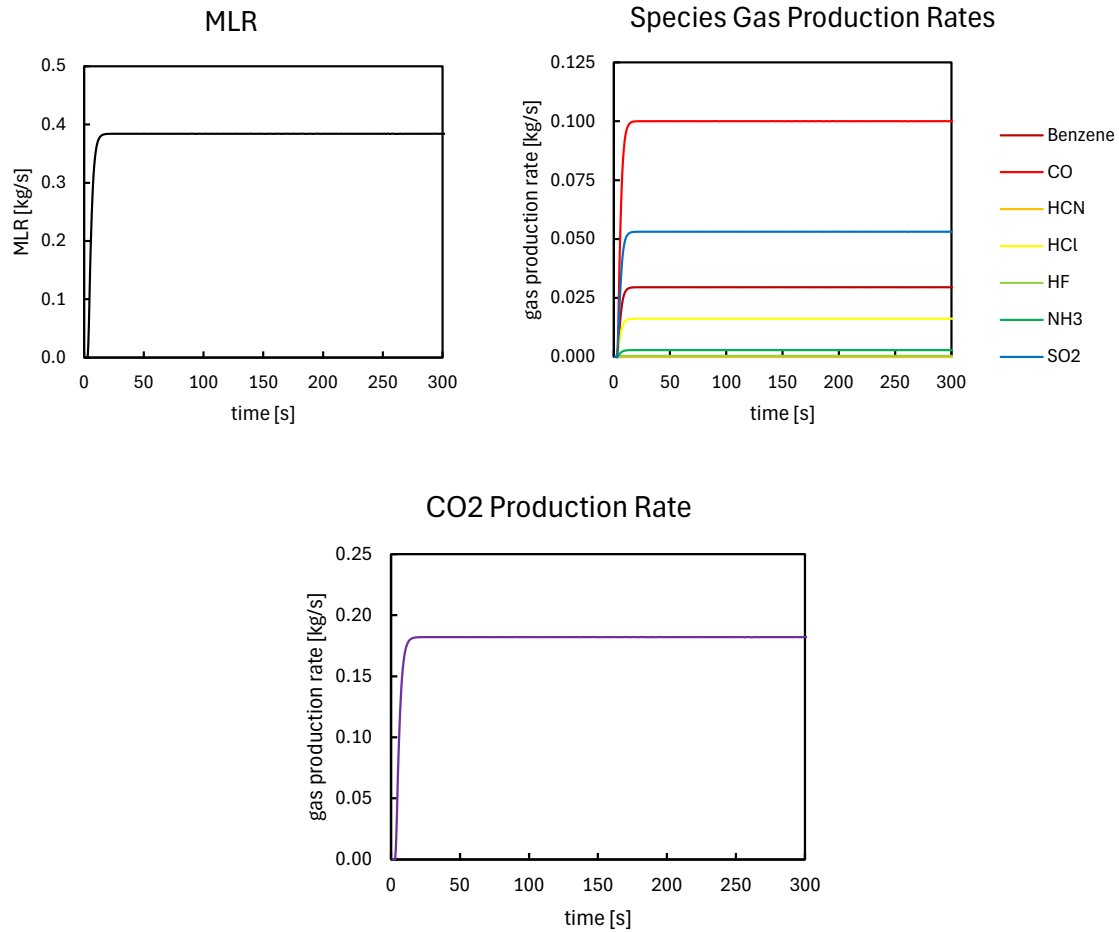


Figure 7. MLR and species gas production rates from FDS/Pyrosim for the NMC non-flaming scenario at a 0.5-hour incident duration.

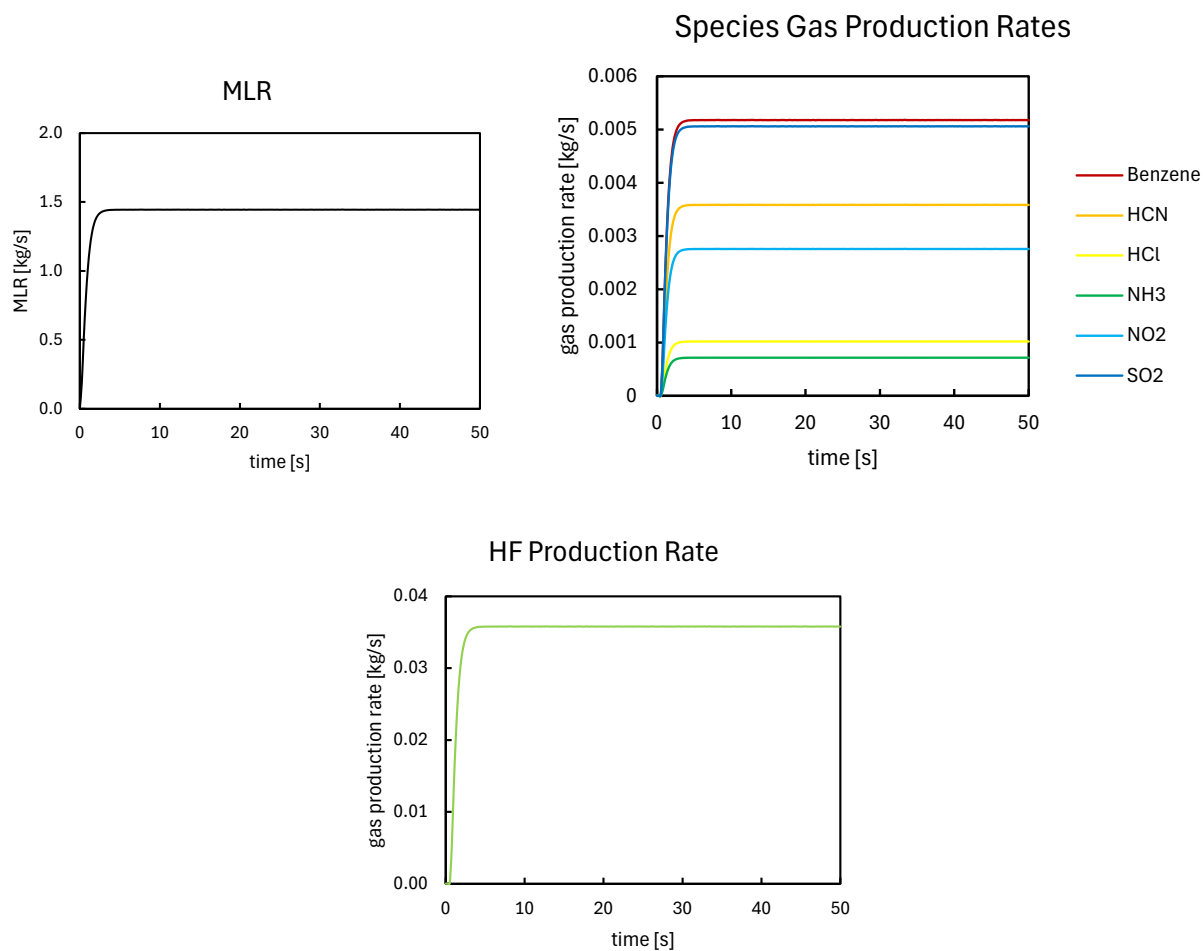


Figure 8. MLR and species gas production rates from FDS/Pyrosim for the LFP flaming scenario at a 2-hour incident duration.

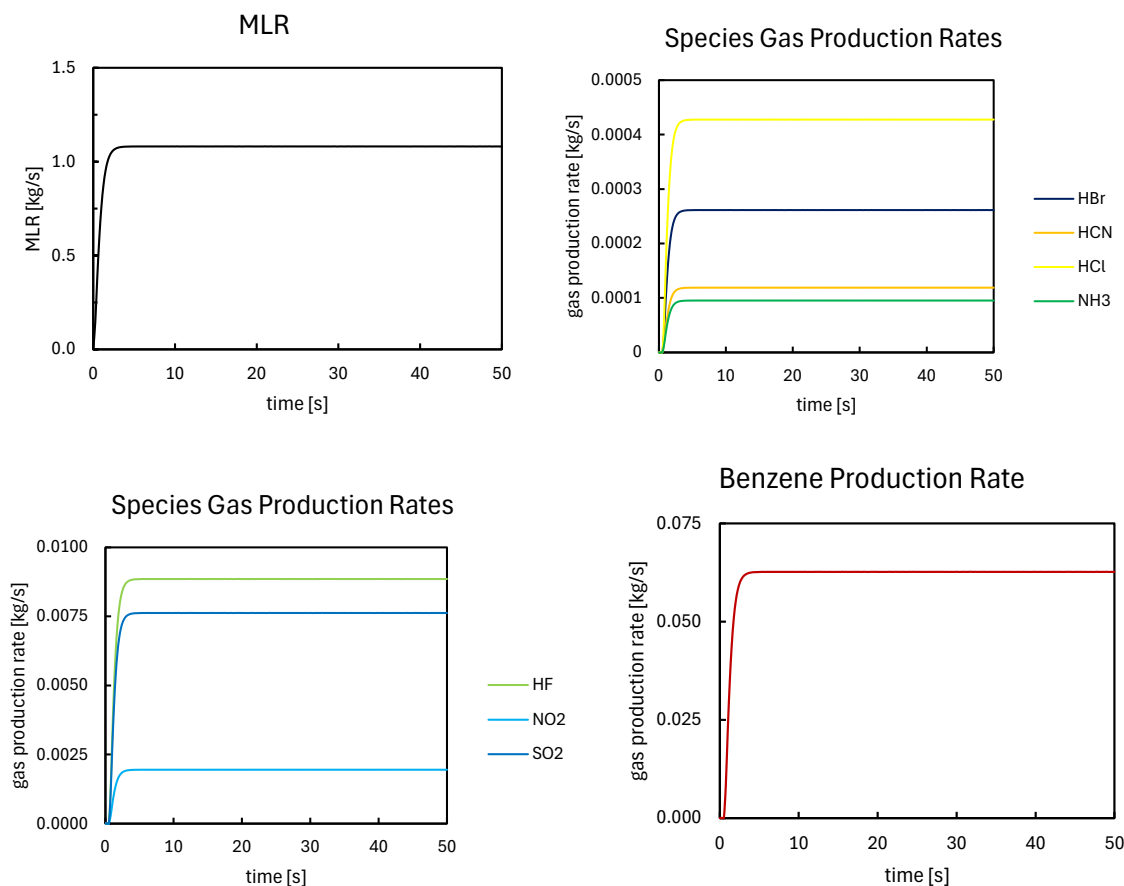


Figure 9. MLR and species gas production rates from FDS/Pyrosim for the NMC flaming scenario at a 2-hour incident duration.

The full list of health impact exposure limit distances (measured from the downwind edge of the BESS unit) for each scenario is provided in Appendix 7.5. Exposure limit distances evaluated by AEGL concentrations are always further than IDLH distances due to the more conservative nature of AEGL limits. Across all factors (non-flaming vs. flaming, cell chemistry, wind, temperature, and duration), CO₂ is the only gas that remained below both IDLH and AEGL/ERPG/TEEL-1 concentrations outside the BESS unit.

The furthest IDLH distance for LFP, non-flaming, is 70 m and is produced by NO₂ under a 5 m/s wind speed at 35°C for a 6-hour duration incident. The furthest AEGL-1 distance for LFP non-flaming exceeds the length of computational domain (200 m) and is produced by NO₂ under all wind speeds, ambient temperatures, and incident durations. The furthest IDLH distance for NMC non-flaming is 81 m and is produced by HCl under a 10 m/s wind speed at 22°C for a 0.5-hour duration incident. The furthest AEGL-1 distance for NMC non-flaming exceeds the length of the computational domain (200 m) and is produced by HCl under a 5 and 10 m/s wind speeds at all temperatures for all incident durations. Figure 10 through Figure 13 present the FDS/Pyrosim concentration plots for the non-flaming cases that produced the furthest distances assessed by occupational and community exposure limits. The maximum value of the color scale in the plots below is set equal to the evaluated exposure limit. As such, concentrations within the red

highlighted areas may be greater than the exposure limit. The views are taken from top down at a height of 1.5 m (breathing height).

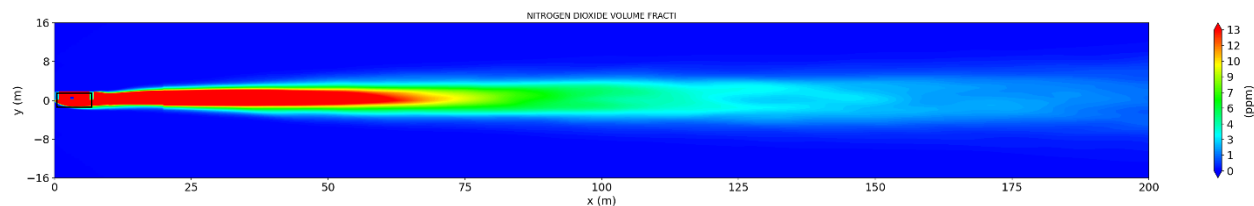


Figure 10. LFP non-flaming NO₂ IDLH concentrations at 2 m/s, 35°C, and 6-hour duration.

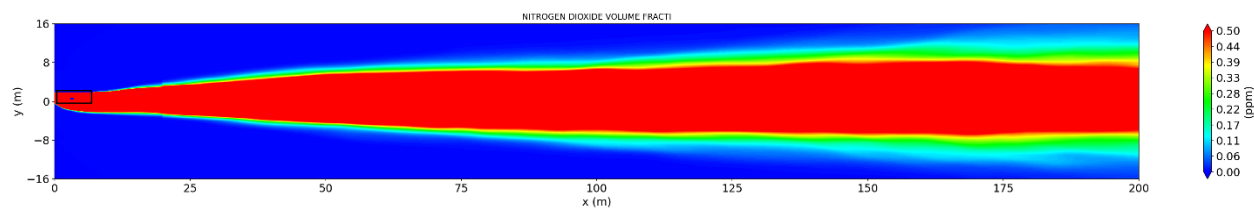


Figure 11. LFP non-flaming NO₂ AEGL-1 concentrations at 2 m/s, 22°C, and 6-hour duration.

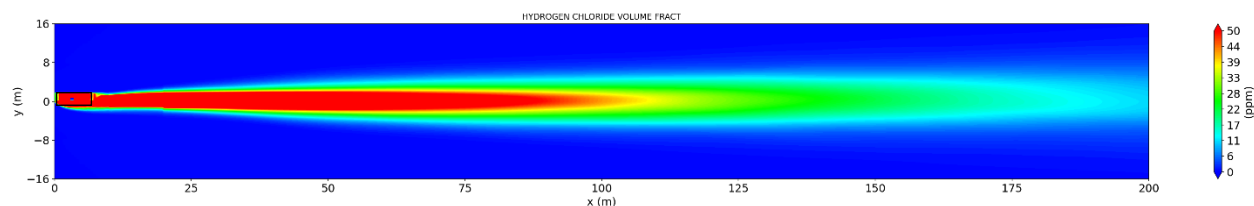


Figure 12. NMC non-flaming HCl IDLH concentrations at 10 m/s, 35°C, and 0.5-hour duration.

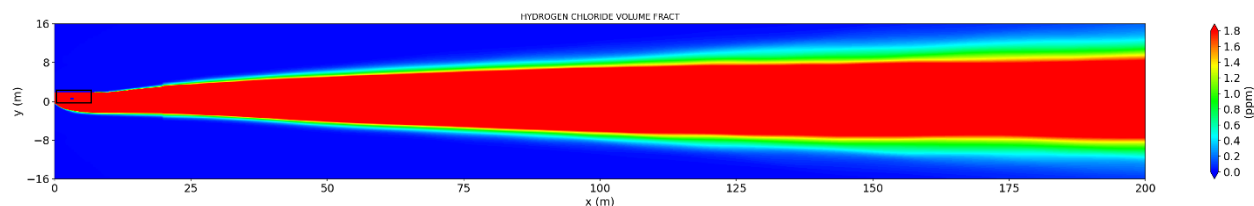


Figure 13. NMC non-flaming HCl AEGL concentrations at 5 m/s, 22°C, and 0.5-hour duration.

The furthest IDLH distance for LFP flaming is 1.125 m and is produced by HF under a 10 m/s wind speed at 22 and 35°C for a 2-hour duration incident. The furthest AEGL-1 distance for LFP flaming is 16 m and is produced by HF under a 10 m/s wind speed at 22°C for a 4-hour duration incident. The furthest IDLH distance for NMC flaming is 1 m and is produced by HF under a 10 m/s wind speed at 7, 22, and 35°C for a 2-hour duration incident. The furthest AEGL-1 distance for NMC flaming is 15 m and is produced by SO₂ under a 10 m/s wind speed at 35°C for a 6-hour duration incident. Figure 14 through Figure 17 present the FDS/Pyrosim concentration plots for the flaming cases that produced the furthest distances assessed by occupational and community exposure limits.

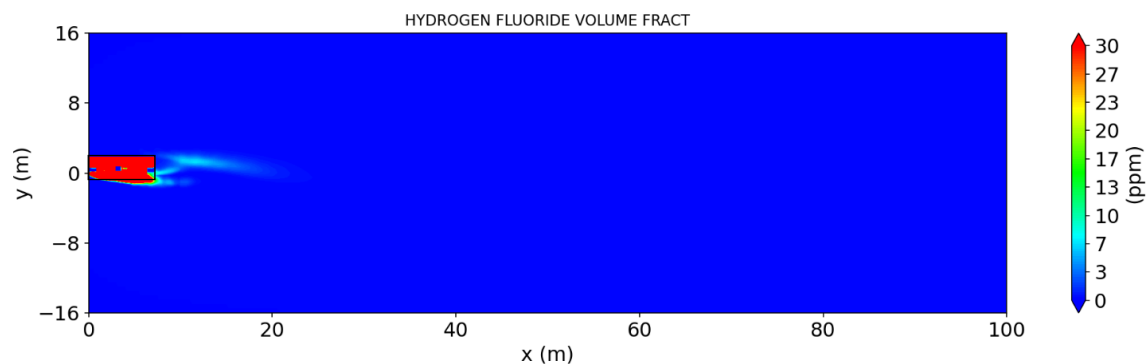


Figure 14. LFP flaming HF IDLH concentrations at 10 m/s, 22°C, and 2-hour duration.

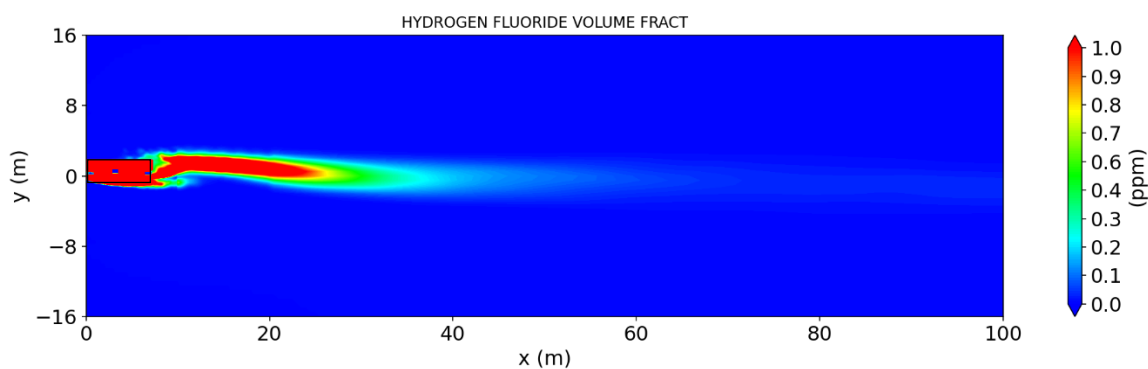


Figure 15. LFP flaming HF AEGL-1 concentrations at 10 m/s, 22°C, and 4-hour duration.

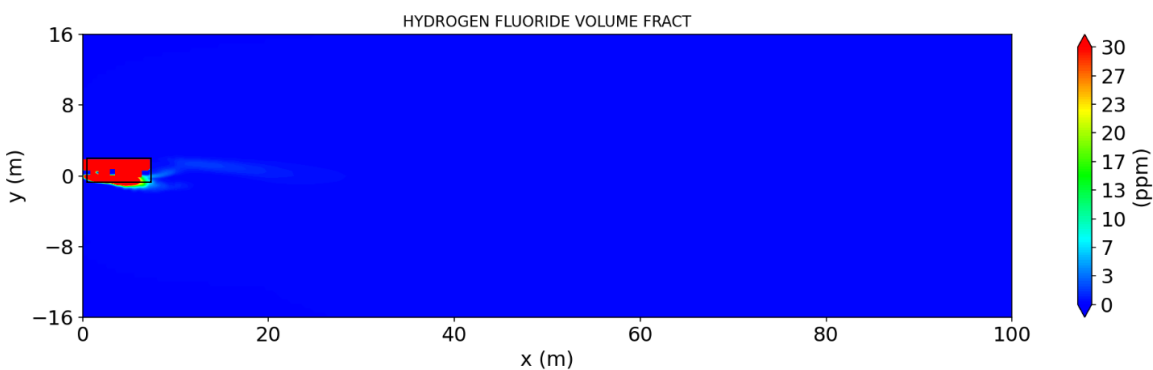


Figure 16. NMC flaming HF IDLH concentrations at 10 m/s, 7°C, and 2-hour duration.

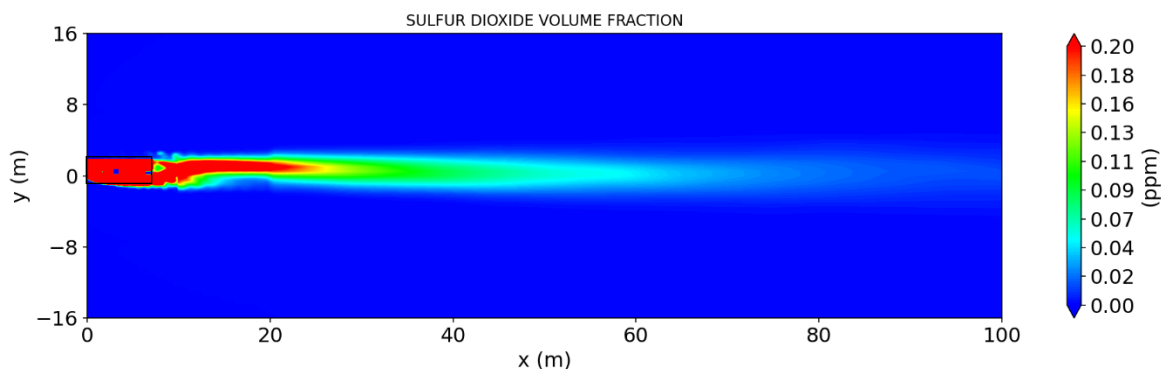


Figure 17. NMC flaming SO₂ AEGL-1 concentrations at 10 m/s, 35°C, and 6-hour duration.

The flaming and non-flaming concentrations above represent the worst-case scenario for occupational and community exposures using the given methodology and data sets. While Figure 14 and Figure 16 show the furthest distances for the flaming LFP and NMC evaluated at IDLH, all distances evaluated at IDLH are within half a meter of each other. These minimal IDLH distances are due to the fact that the BESS unit vents, where gas release occurs, are located at the top of the enclosure (elevation of 2.5 m), which is higher than the breathing height elevation of 1.5 m. With the high buoyancy of the plume, minimal gases drop down to the breathing height elevation. The proceeding sections discuss the factors that impact exposure limit distances; these factors should be considered when conducting a site-specific hazard evaluation.

5.1.1. Factors Affecting Non-Flaming Exposure Limit Distance

The constituents evaluated for the LFP non-flaming scenarios were benzene, CO, CO₂, HCl, HCN, HF, and NO₂. Of these gases, benzene, CO, CO₂, HCl, and HCN never reached IDLH limits outside the BESS unit. Additionally, CO₂ never reached the TEEL-1 limit for the LFP scenarios. The constituents evaluated for the NMC flaming scenarios were benzene, CO, CO₂, HCl, HCN, and HF. Of these gases, CO₂, HCl, and HCN never reached IDLH limits outside the BESS unit. HCN never reached the AEGL-1 limit, and CO₂ never reached the TEEL-1 limit outside the BESS unit for the NMC scenarios.

Overall, the furthest distances determined by community exposure limits for the LFP simulations are larger than the furthest distances for the NMC simulations. The average gas production rate for NMC (207 L/s) is two orders of magnitude higher than the LFP average gas production rate (6 L/s) due to the higher total gas production from NMC cells and the shorter duration over which the gases are released. Gas production rates for benzene, CO, CO₂, HCl, and HF are higher in the NMC cells. However, only benzene and CO distances for the NMC simulations are further than distances for the LFP simulations. This can be attributed to the difference in plume development. Figure 18 and Figure 19 present the plume development in FDS/Pyrosim for the LFP and NMC non-flaming scenarios under a 2 m/s wind speed at 22°C for a 6-hour and 0.5-hour incident duration, respectively. An artificial soot density was added to the non-flaming scenarios to aid in visualization of the smoke plume. It is expected that a plume from a non-flaming thermal runaway condition would be opaque, as soot is not produced during non-flaming conditions.



Figure 18. LFP non-flaming plume at 2 m/s, 22°C, and 6-hour duration.



Figure 19. NMC non-flaming plume at 2 m/s, 22°C, and 0.5-hour duration.

As shown above, the LFP plume is closer to breathing height compared to the NMC plume. This is attributed to the lower average cell venting temperature of LFP cells compared to NMC cells, which decreases buoyancy of the plume in the LFP scenarios. Benzene and CO have gas production rates that are one order and two orders of magnitude, respectively, above the LFP production rates; the increased production rates overcame the impact caused by the buoyancy of the NMC plume at breathing height.

Higher constant ambient temperatures consistently increase the furthest distance that both occupational and community exposure limits are reached. All non-flaming worst-case scenarios were produced from simulations with a 35°C ambient temperature. Although it was expected that the higher wind speeds would produce long distances, this was not the case for the non-flaming scenarios. The wind speed that produces the furthest exposure limit distance for LFP is dependent on species, incident duration, temperature, and the type of exposure limit. When evaluated at IDLH, HF and NO₂ tend to produce further distances at the 5 m/s wind speed in the 6-hour duration simulations, whereas the 2 m/s wind speed produces further distances in the 12-hour duration simulations. However, HF produces further distances at 5 m/s regardless of incident duration when evaluated at AEGL-1. CO follows a similar pattern, although none of the 12-hour incident duration simulations reach ERPG-1 limits outside of the BESS unit. The reason the lower wind speeds (2 m/s and 5 m/s) cause concentrations to exceed exposure limits at a further distance may be due to the plume density. As shown in Figure 18 and Figure 19, the LFP non-flaming plume is closer to the ground and less dense compared to the NMC plume. Figure 20 presents the LFP non-flaming scenario under a 10 m/s wind speed at 22°C for a 6-hour incident duration in FDS/Pyrosim.

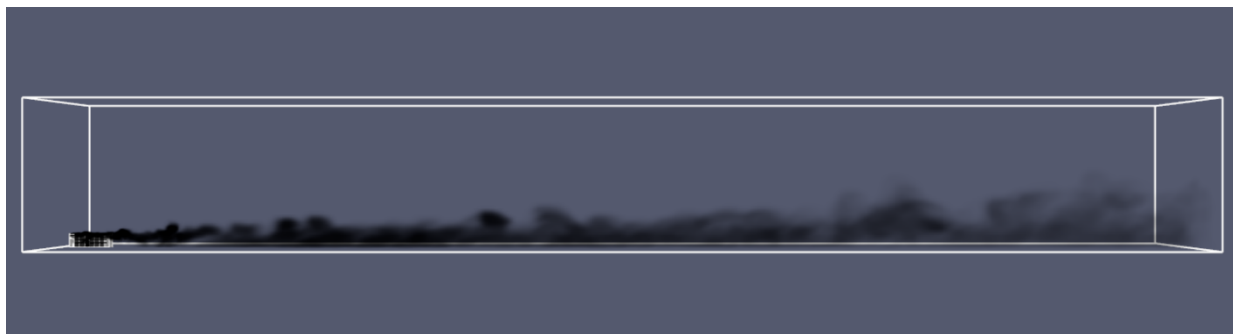


Figure 20. LFP non-flaming plume at 10 m/s, 22°C, and 6-hour duration.

When comparing the 2 m/s and 10 m/s scenarios, the plume is more dispersed in the 10 m/s scenario. The already low buoyancy and density that characterizes the LFP non-flaming plume allows the plume to be dispersed more readily at higher wind speeds. At the 10 m/s wind speed, the LFP non-flaming plumes have dispersed too much to reach concentrations that exceed exposure limits, despite the plume being closer to breathing height. Since the 12-hour incident duration simulations release gas at a lower rate, the plume is more likely to disperse at a 5 m/s wind speed compared to the 6-hour incident duration simulations.

When evaluated at community exposure limits, HCl and benzene tend to produce further distances at the 5 m/s wind speed in the 6-hour duration simulations and at the 2 m/s wind speed in the 12-hour duration simulations. HCN follows a similar pattern at lower temperatures (7°C). At higher temperatures (22°C and 35°C), HCN tends to produce further distances at 2 m/s regardless of duration. It is possible that the different trends between each species are due to the varying molecular weight; however, the exact effect is unclear. More research is required to see how molecular weight impacts concentrations at lower gas production rates.

For the NMC simulations evaluated at community exposure limits, the 0.5-hour duration simulations produce further distances at the 10 m/s wind speed, whereas the 5 m/s wind speed produces further distances for the 2-hour duration simulations. The 2 m/s wind speeds always produce the shortest distance for the NMC simulations. HF and benzene barely reach IDLH concentrations outside of the BESS unit (0.25 m). Only CO levels reach IDLH limits at a significant distance and follow the same pattern as the community exposure limits, except at 35°C for the 0.5-hour incident duration simulations.

The effects of different incident durations on which wind speed produced the furthest distance is due to the difference in gas release rates. In the 0.5-hour incidents, the gas release rate, and thus plume density, are high enough to overcome mixing and dispersion effects caused by the high wind speeds. Therefore, the plume can remain concentrated for a greater horizontal distance. In the 2-hour incidents, the lesser gas release rate causes a less dense plume that is more easily mixed and dispersed, especially at high wind speeds (i.e., 10 m/s). However, at moderate wind speeds (i.e., 5 m/s), the horizontal transport effects of the wind still outweigh the mixing and dispersion effects. Figure 21 presents the plume development in FDS/Pyrosim for the NMC non-flaming scenario under a 2 m/s wind speed at 22°C for a 0.5-hour incident duration.



Figure 21. NMC non-flaming plume at 2 m/s, 22°C, and 2-hour duration.

Compared to the 0.5-hour incident duration plume, the 2-hour incident duration plume is closer to the ground and less buoyant. This causes the 2-hour incident duration plume to disperse more readily and behaves similarly to the LFP non-flaming plume. The 0.5-hour plume has a higher gas release rate that allows the plume to maintain its shape and buoyancy. Thus, the primary factor controlling exposure limits is the wind which can push the plume to breathing height.

5.1.2. Factors Affecting Flaming Exposure Limit Distance

The constituents evaluated for the LFP flaming scenarios are CO, CO₂, HCl, HF, NH₃, NO₂, and SO₂. Of these gases, CO, CO₂, HCl, NH₃, and SO₂ never reach IDLH limits outside the BESS unit. CO, CO₂, HCl, and NH₃ never reach community exposure limits for the LFP scenarios. The constituents evaluated for the NMC flaming scenarios are benzene, CO, CO₂, HBr, HCl, HCN, HF, NO₂, and SO₂. Of these gases, benzene, CO, CO₂, HBr, HCl, and HCN never reach IDLH limits outside the BESS unit. CO₂, HCl, and HCN never reach community exposure limits for the NMC scenarios.

In general, the LFP and NMC flaming cases produce similar furthest distances. The LFP cell chemistry produces higher total MLRs compared to the NMC cell chemistry. Species production for HF, CO, CO₂, HCl, NO₂, HCN, and NH₃ are higher for the LFP cell chemistry. However, the gas concentrations in the plume had less impact on the furthest distance compared to the plume development and effect of wind. Figure 22, Figure 23, and Figure 24⁸ provide the plume development for the LFP flaming scenario under a 2, 5, and 10 m/s wind speed, respectively, at 22°C for a 2-hour incident duration. The NMC and LFP flaming plumes have similar profiles in FDS/Pyrosim. The plume development for the 2 m/s wind scenario appears to flatten at the mesh boundary; however, running the simulation with a taller domain shows that the plume continues to rise and bends sideways approximately at the mesh domain.

⁸ The plumes displayed in these figures are not intended to visually represent the color and density of plumes produced by BESS fires but are used to visualize the plume direction and dispersion.



Figure 22. LFP flaming plume at 2 m/s, 22°C, and 2-hour duration.



Figure 23. LFP flaming plume at 5 m/s, 22°C, and 2-hour duration.



Figure 24. LFP flaming plume at 10 m/s, 22°C, and 2-hour duration.

As shown above, the proximity of the plume to breathing height is significantly affected by the increase in wind speed. Both the LFP and NMC simulations produce similarly buoyant plumes. As expected, the higher wind speeds push the plume down further, resulting in further occupational and community exposure limit distances. All worst-case scenarios for the flaming cases are produced at the 10 m/s wind speed, regardless of temperature or cell chemistry. Increases in incident duration tends to decrease the distance at which exposure limits were exceeded but does not have as pronounced effect compared to wind speed. Changes in ambient temperature have little effect.

5.1.3. Comparison Between Non-Flaming and Flaming Cases

The non-flaming cases produce further distances at which concentrations exceeded exposure limits at breathing height compared to the flaming cases, despite the overall higher toxic gas concentrations in flaming plumes. This is due to the difference in buoyancy between the two cases. The non-flaming plumes have a lower MLR and temperature, causing them to have a closer proximity to breathing height. Conversely, the flaming plume is too buoyant to sink closer to the ground and escapes the vertical domain entirely. Since the plume escapes the vertical computational domain, the highest concentrations of toxic gases do not reach breathing height. The flaming plumes have the potential to begin dispersing further away from the BESS unit, despite having smaller exposure limit distances compared to the non-flaming plume. For the non-flaming cases, the plume does not escape the vertical domain, and most toxic gases disperse within the computational domain. As such, it is unlikely that the non-flaming plumes will disperse much further outside of the computational domain, apart from the NMC non-flaming scenarios with a 2-hour incident duration. In most non-flaming cases, the plume mixes with air as it travels and continues to disperse within the domain. AERMOD was utilized to explore whether the flaming and non-flaming cases would produce concentrations exceeding PACs exposure limits in the far-field.

The impact of different factors is more apparent with the non-flaming scenarios. While wind is the main controlling factor in exposure limit distances for the flaming scenarios, the non-flaming scenarios vary significantly by all factors. Cell chemistry, temperature, and species, which significantly change the trends in the non-flaming cases, have little impact in the flaming cases. Additionally, duration has a larger impact on exposure limit distances in the non-flaming scenarios compared to the flaming scenarios.

5.2. *AERMOD*

5.2.1. Health Impact Quantification

The full list of health impact exposure limit distances for each scenario are provided in Appendix 7.5. For the LFP non-flaming scenario at a 6-hour incident duration, the furthest AEGL-1 distance is 322 m and is produced by NO₂. For the NMC non-flaming scenario at a 0.5-hour incident duration, the furthest AEGL-1 distance is 418 m and is produced by HCl. For the LFP flaming scenario at a 4-hour incident duration, the furthest AEGL-1 distance is 83 m and is produced by HF. For the NMC flaming scenario at a 4-hour incident duration, the furthest AEGL-1 distance is 62 m and is produced by SO₂. Figure 25 to Figure 28 show the concentration plots for the cases that produced the furthest distances assessed by community exposure limits in AERMOD.

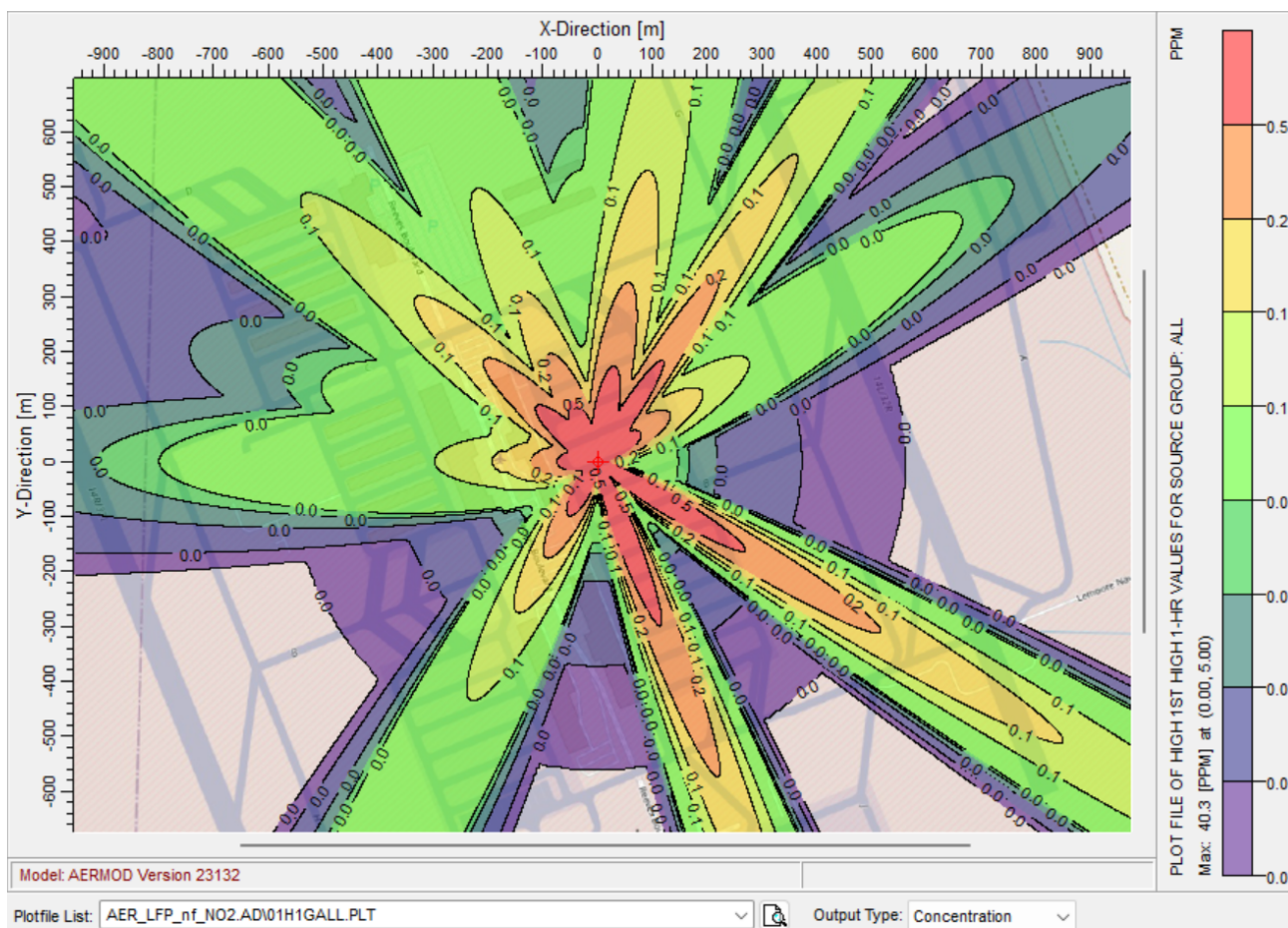


Figure 25. NO₂ AERMOD concentration plot for the LFP non-flaming scenario.

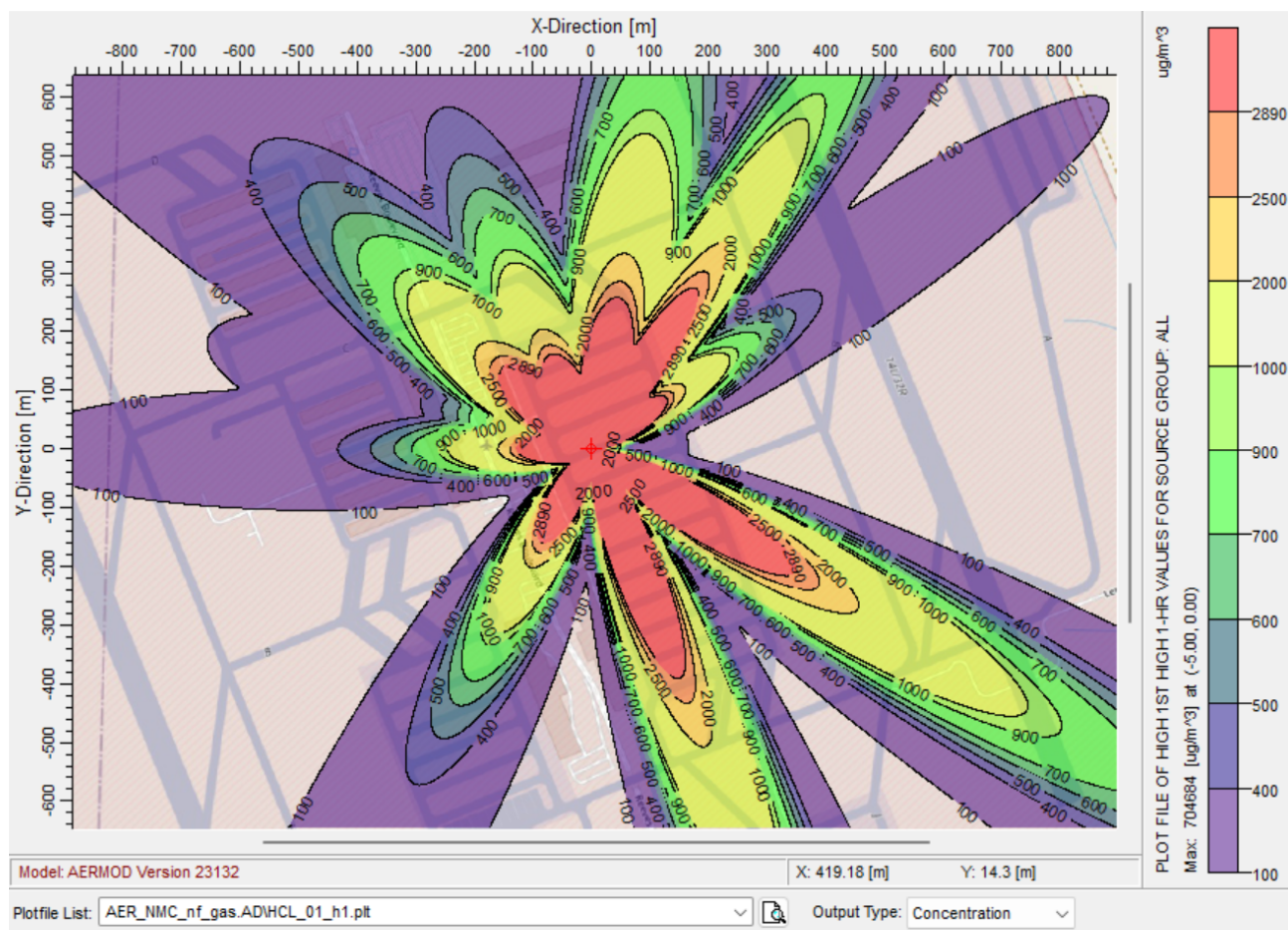


Figure 26. HCl AERMOD concentration plot for the NMC non-flaming scenario.

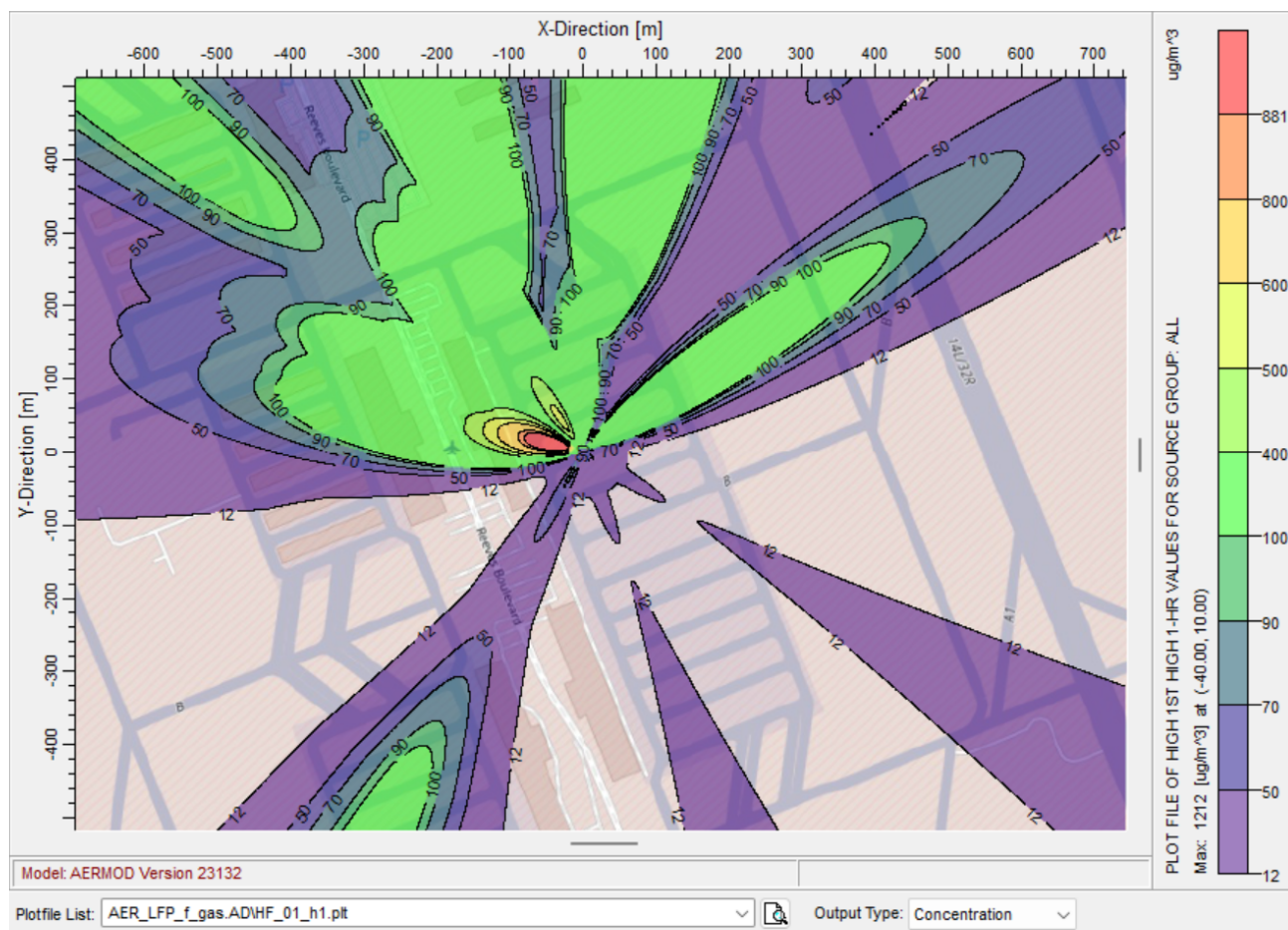


Figure 27. HF AERMOD concentration plot for the LFP flaming scenario.

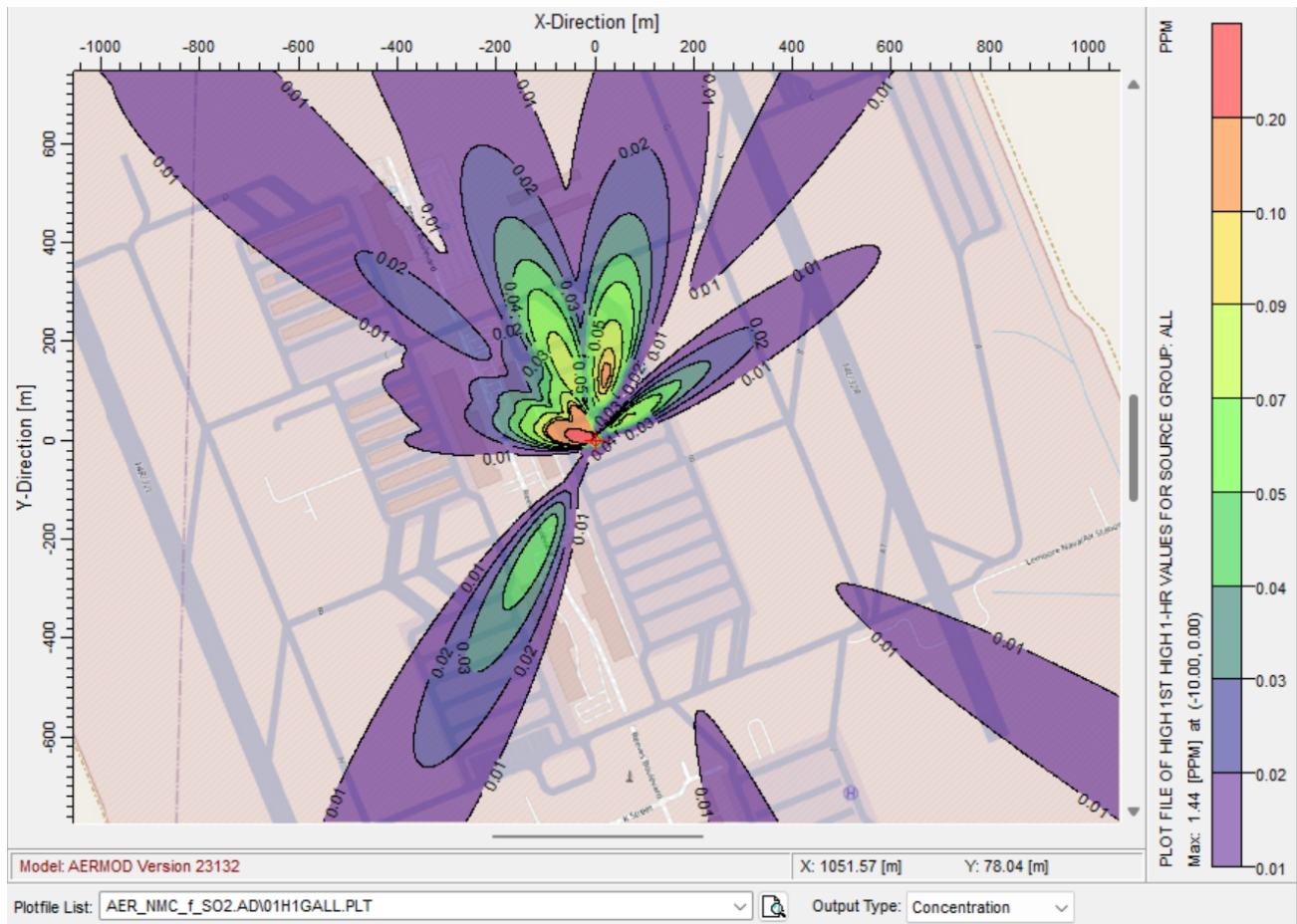


Figure 28. SO₂ AERMOD concentration plot for the NMC flaming scenario.

The same constituents that produced the furthest community exposure limit distances in FDS also tended to produce the furthest distances in AERMOD. The gases that produced larger exposure limit distances tended to have higher emission rates compared to other gases with similar community exposure limits. Gases such as benzene, CO, CO₂, and NH₃ had higher community exposure limit concentrations, so regardless of the higher emission rates, these constituents do not produce the furthest exposure distances.

The flaming AERMOD simulations show plume rise and grounding, whereas the non-flaming scenarios consistently decrease radially from the BESS unit. While the flaming plume spreads further due to buoyancy, it does not produce high enough concentrations to reach community exposure limits within the domain. The non-flaming exposure limit distances produced in AERMOD are similar to those produced in FDS. The flaming scenarios produced a larger furthest exposure limit distance compared to the FDS simulations, which is most likely due to the different modeling algorithms that AERMOD uses to account for buoyancy and weather. AERMOD provides a worst-case scenario for the flaming scenarios as modelling rise and subsequent grounding would result in lower concentrations at the same distances due to the mixing and dispersion that occurs during transport.

5.2.2. Environmental Impact Quantification

To conduct a proper environmental impact evaluation, the relevant stakeholder or user would need to determine the relevant locations and ecosystem of interest. For the purposes of this study, it was assumed that the BESS source is 1.0 km north from Kings River. Total surface deposition calculated in AERMOD at this location was 0.04747 g/m^2 . Figure 29 shows the total surface deposition from the BESS unit.

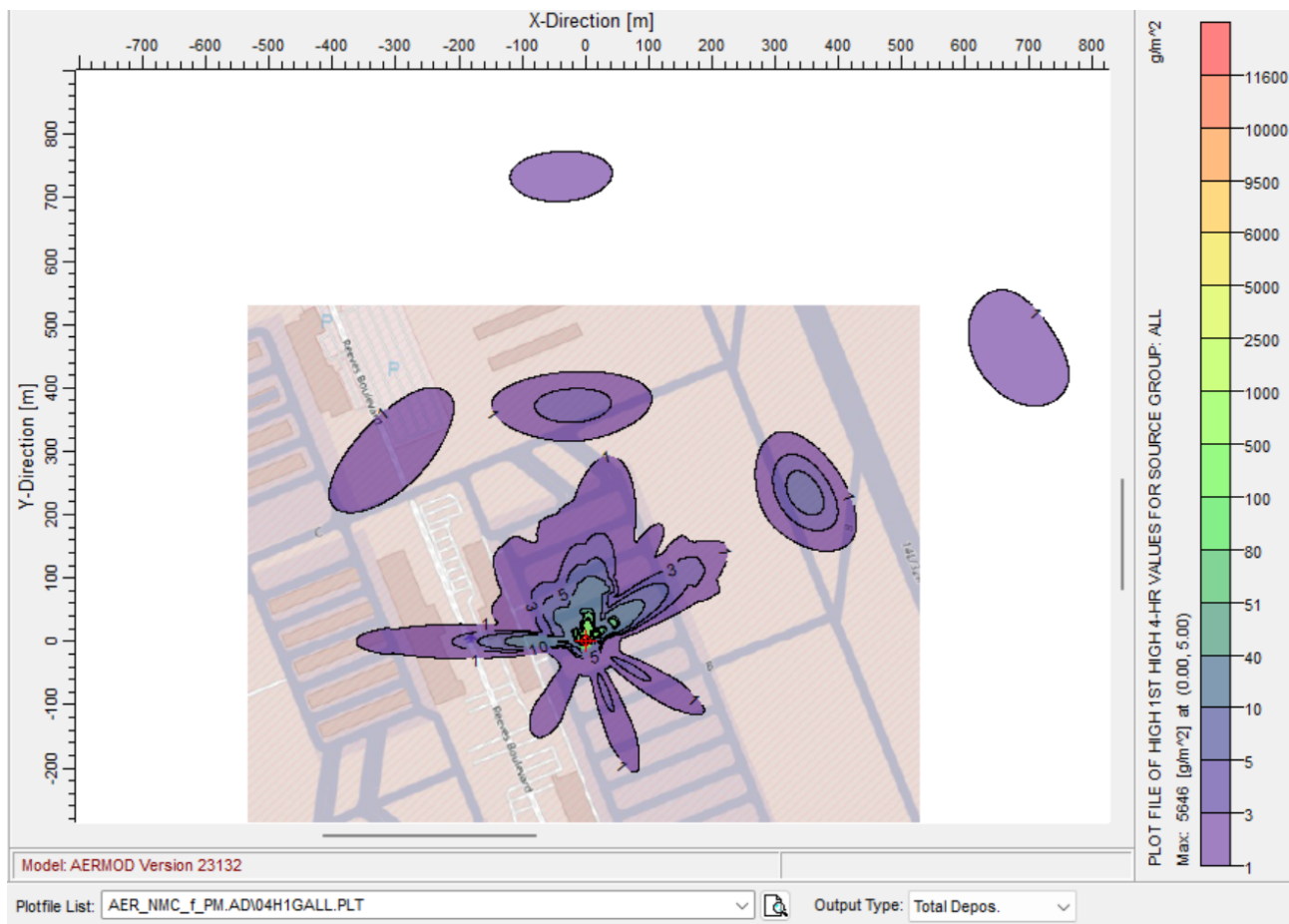


Figure 29. Total surface deposition for the NMC flaming scenario.

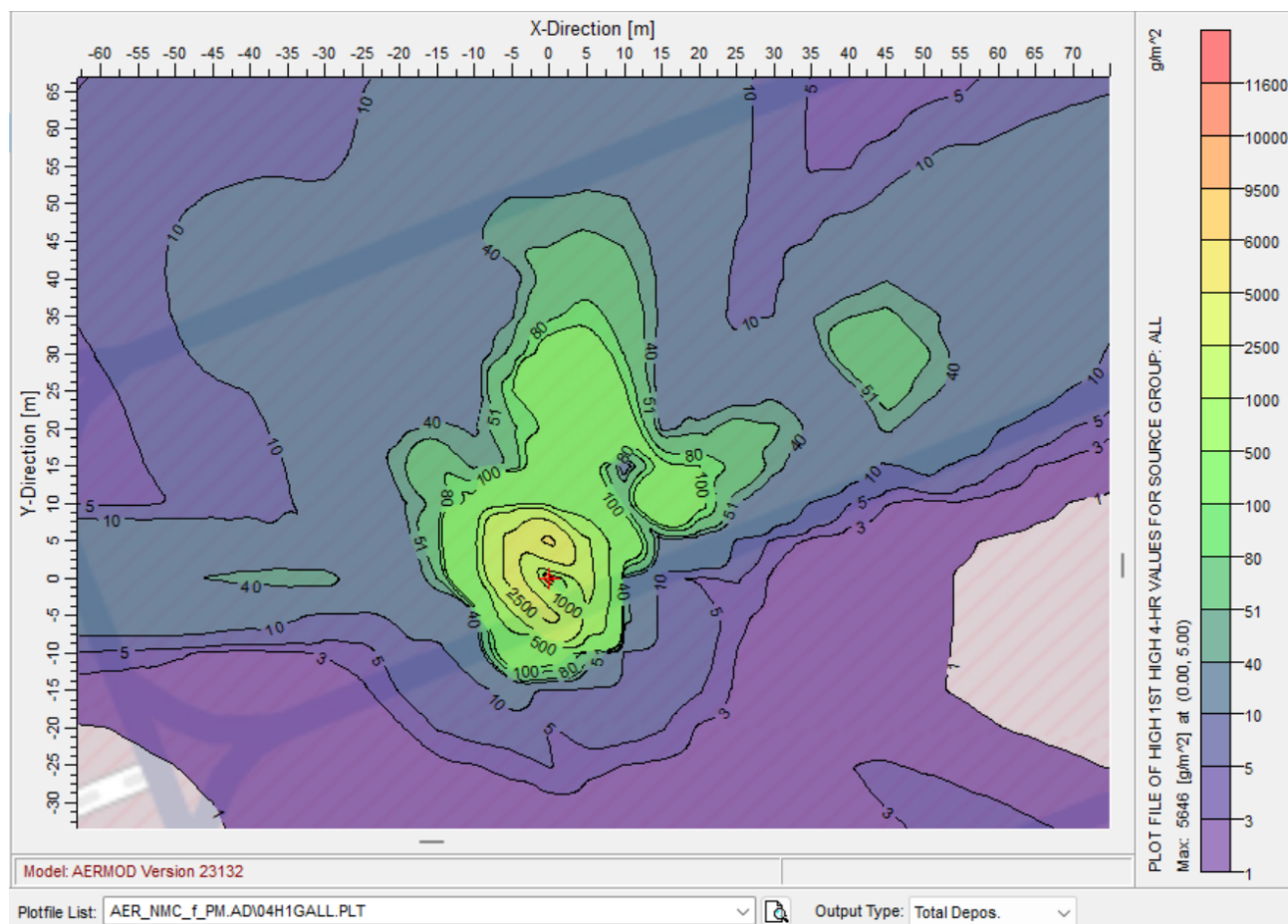


Figure 30. Total surface deposition nearby the BESS unit for the NMC flaming scenario.

The concentration by volume was calculated by dividing total surface deposition by reference depth. The concentration of particulate matter in soil is 0.625 mg/L, and the concentration of particulate matter in water is 0.010 mg/L. Concentrations for each metal were calculated by multiplying total deposition with the percent mass composition shown in Table 22. Metal concentrations in soil and water from plume deposition are presented in Table 32.

Table 32. Metal concentrations for the NMC non-flaming scenario.

Environment	Concentration [mg/L]					
	Li	Ni	Co	Mn	Al	Cu
Soil	0.0219	0.1562	0.0581	0.0500	0.0394	0.0337
Water	0.0003	0.0024	0.0009	0.0008	0.0006	0.0005

None of the constituents exceeded the exposure limit guidelines, indicating that the earthworms and aquatic species located 1.0 km north of the BESS unit would not be impacted in the modeled scenario.

The lowest earthworm EC_{50} value is for lithium at 22.4 mg/L. In order to reach this EC_{50} value, the total surface deposition from the plume would have to be 51 g/m² or greater at the evaluated

area. The lowest green algae EC_{50} value is for aluminum at 150 mg/L. In order to reach this LC_{50} value, the total surface deposition from the plume would have to be 11600 g/m² or greater at the evaluated area. As shown in Figure 29, concentrations at 51 g/m² are confined to within 60 m of the BESS unit. Total deposition does not reach 11600 g/m².

5.3. Environmental Impact via Water Runoff

To estimate the potential starting concentrations of contaminants in water at the fire source, it was necessary to normalize and scale the results found in the literature to a large-scale BESS incident. Bordes et al. (2024) used a historical incident in France involving a 1,500 kWh BESS unit, where the fire department estimated a total volume of 180,000 liters of water was applied (0.12 L/Wh), to extrapolate their experimental data and compare to European regulatory thresholds for fresh water [109]. Using the same methodology and estimates for the amount of water that may be applied during an incident involving a large-scale, outdoor BESS unit, Table 33 presents the average experimental results from Bordes et al. (2024), Held et al. (2022), and Quant et al. (2023), which all utilized NMC cells in their tests [109][110][76]. Long et al. (2013) was excluded, because the tests included interior finishes of a vehicle, and therefore did not exclusively represent contaminants produced by Li-ion cells [111]. The values from the literature were compared to green algae EC_{50} values for organic element from ECOSAR, also indicated in Table 33.

Table 33. Average concentrations of organic elements found in firewater runoff from Li-ion battery thermal runaway compared to EC_{50} values.

Element	Concentration in Water applied at 0.12 L/Wh [mg/L]	EC_{50} for Algae [mg/L]
Al	7	150
Co	5	344
Cr	0.002	304
Cu	0.1	1330
Fe	0.5	1610
Li	54	200
Mn	5	321
Mo	0.1	561
Ni	7	1230
Sb	0.02	329
Chloride	18	154
Fluoride	31	224

The results of this analysis show that significant environmental impacts are not expected as the result of fire water runoff contaminated with metals, fluoride, or chloride. While levels of these elements would be elevated, due to dilution, they are not high enough to cause a significant impact to water-based organisms.

5.4. *Limitations and Future Research*

The scope of this methodology is limited to the health and environmental impacts contributed by Li-ion cells, modules, and racks of modules. BESS units contain wiring, electronics, plastic components, cooling liquid, etc. that can contribute to the production of toxic gases and metal particulate. These components are manufacturer specific and can be evaluated if the structure of the BESS unit is known. Contributions from all components found in a unit were not evaluated in this study, as there is insufficient data to fully characterize the mass percentage of all components in the product's finished, fully functional form. This methodology is not meant to be conducted during an incident and will not be able to provide immediate results.

Google Scholar was the only search engine utilized in this study. However, it has limited search results and certain articles were not available due to paywall or language barriers, which reduced the range of articles included in this study. To supplement Google Scholar, other search engines such as Web of Science or Scopus can also be utilized.

Health impact was quantified through inhalation of individual toxic and irritant gases; however, simultaneous exposure to multiple toxic gases or irritant gases can have an additive health effect, respectively [112]. This additive effect is often evaluated with the concept of Fractional Effective Concentration or Dose (FEC or FED) which is used to estimate the accumulated dose of multiple toxic gases, as a fraction of the dose required to produce a given effect, such as cause collapse and loss of consciousness. While this concept is useful for prediction of irreversible or serious health effects, such as those that may occur at AEGL/ERPG/TEEL Level 2 or 3 thresholds, it is not generally applied for transient and reversible health effects, such as those that may occur at AEGL/ERPG/TEEL Level 1 thresholds (i.e., irritation, discomfort). The evaluation of community exposures in this study was based on AEGL/ERPG/TEEL Level 1 thresholds, therefore, additive effects from exposure to multiple toxic gases simultaneously were not considered. Regarding occupational exposures (i.e., emergency personnel), the IDLH thresholds used for evaluation are associated with irreversible or serious health effects. Therefore, if these individuals are expected to be exposed to higher plume concentrations for other than instantaneous durations, consideration of additive effects is likely important. However, the use of self-contained breathing apparatus (SCBA) by emergency personnel within the near vicinity (<100 m) of the BESS unit would protect against these toxic gas exposures and health effects. As such, this study did not consider additive health effects for occupational exposures. In addition to inhalation of toxic gases, there are other fire plume hazards that may cause adverse health effects. Thermal runaway of BESS units has the potential to disperse airborne metal particulates and other particulate matter. This study did not evaluate the health hazards of these constituents through respiration, ingestion, or absorption. To perform such an evaluation, additional data on the yields, size distribution, and composition of respirable particles (<10 μm) is needed; there is limited data on this issue.

Environmental impact was confined to soil and surface freshwater. No evaluation of impact to air was performed. Additionally, the environmental impact focused on acute exposure. However, the deposited metal particulates can remain in the soil and water for an extended period of time and/or reach groundwater; though soil and water concentrations will decrease during this time due to dilution, migration, leaching, etc. The persistence of these elements, final destinations, and the rate at which they decrease or migrate is dependent on the topography, body of water, and meteorological conditions, and would need to be evaluated on a case-by-case basis by the relevant stakeholder or user in collaboration with an environmental professional.

Compared to the HRR estimates calculated with data from the literature review, the FDS model overpredicted HRR for the LFP flaming cases and underpredicted HRR for the NMC flaming cases. This was due to the default use of oxygen consumption calorimetry in FDS instead of a specific heat of combustion representative of Li-ion cells. The difference in the overprediction/underprediction of HRR between the LFP scenarios and the NMC scenarios was due to the difference in the combustion reactions utilized, i.e., LFP combustion was modeled with a greater methane fuel ratio. A lower modeled HRR in the LFP scenarios would produce a less buoyant plume, and therefore gas concentrations at breathing height would be expected to increase. Conversely, a higher modeled HRR in the NMC scenarios would produce a more buoyant plume, and therefore gas concentrations at breathing height would be expected to decrease. However, despite differences in HRR, the LFP and NMC simulations produced similarly buoyant plumes. As such, the variances in modeled HRR versus calculated HRR, are not expected to have a significant impact on the trends and conclusions of this study. Improved balancing of the MLR, HRR, and gas yields via the combustion reaction specifications is recommended in a specific hazard analysis to ensure more accurate representation of each of these factors.

The full range of chemical reactions that can occur within the plume as it travels are not simulated in AERMOD or FDS. Ambient temperature and relative humidity can impact chemical kinetics. In addition, toxic gases, like HF, can react with wet and dry surfaces including water molecules within the air. HF is particularly reactive and highly soluble, with fluorine deposition from the atmosphere to surfaces being the dominant mechanism for removal of fluorine from air [80]. At low concentrations, e.g., 10 ppmv, the effects of HF reactivity can be considered negligible, and HF can be treated as inert in an atmospheric transport model; however, at higher concentrations (e.g., kg/s release rate and thousands of ppm), the reactions of HF become important and determine the plume's thermodynamics and behavior [80].

The results of this study show that the concentrations of HF within the plume, and close to the source, can be in the order of magnitude of thousands of ppm. In comparison, the concentrations of HF near the ground level are less than 30 ppm, other than in the very immediate vicinity of the source. Additionally, the maximum HF release rate utilized in the models was 35.8 g/s. Given this release rate, the impact of HF reactivity on the plume behavior, especially regarding grounding and dispersion near the ground, is expected to be minimal. Transfer of fluorine from the air to surfaces is still expected but using an assumption of no reaction of HF with wet or dry surfaces provides for the most conservative toxic gas evaluation for impacts on human health as this assumes all quantities of fluorine remain in the air. There are modeling programs developed for HF release and dispersion; however, these programs do not account for transport of passive species or reactivity with wet or dry surfaces. If an assessment were to be performed for the health and environmental impact of the fluorine transfer from air to soil and/or water, additional analysis on HF reactions and fluorine deposition rates would need to be conducted.

Other factors, such as relative humidity, precipitation, and topography can influence the results. While the full range of these factors were not explored in this research, it is important to consider how they may impact plume buoyancy and development and associated toxic gas concentrations and exposure limit distances. It should also be noted that while the FDS model was run with an Obukhov length of -100 m to indicate thermal instability, the environmental temperature lapse rate was inadvertently set to 0 °C/m. As such, the ambient temperature of the atmosphere remained constant with height. When the environmental lapse rate is greater than the dry adiabatic lapse rate of the plume, i.e., the plume cools slower than the surrounding atmosphere,

the atmosphere is considered very thermally unstable. If the environmental lapse rate is lower than the moist adiabatic lapse rate of the plume, i.e., plume cools faster than atmosphere, the atmosphere is considered very thermally stable [113]. A thermally neutral atmosphere occurs when there is no heat transfer between the air and the ground [114]. The modeled atmosphere did not cool, so all scenarios were unintentionally modeled in a thermally stable environment. To assess the impact of this factor, three FDS/Pyrosim simulations were run at different temperature lapse rates and stabilities under a 5 m/s wind speed to assess the impact of temperature lapse rate on plume development, as shown in Table 34.

Table 34. Simulation parameters for temperature lapse rate sensitivity analysis.

Stability	Temperature Lapse Rate [K/km]	Obhukov Length [m ⁻¹]
Stable	12	350
Neutral	-10	1,000,000
Unstable	-20	-350

The three scenarios are shown in Figure 31 to Figure 33.



Figure 31. Plume development under a 12 K/km lapse rate.



Figure 32. Plume development under a -10 K/km lapse rate.



Figure 33. Plume development under a -20 K/km lapse rate.

The species gas concentrations of the plume at breathing height did not change significantly between different temperature lapse rates. This is because the height of the FDS domain is 43 m, therefore the change in temperature by height is only by fractions of a degree. While there are some differences between plume development and density, these changes do not occur at breathing height and thus, do not affect the exposure limit distances.

Franqueville et al. (2023) determined that the most impactful parameter to determining exposure limit distances was toxic gas yield [47]. While Franqueville et al. (2023) did not evaluate particulate deposition, it can also be assumed that particulate yield performs a similar function to toxic gas yield. However, there is significant variation in the datasets available. A comprehensive data set of toxic gas yield was not available from any one literature source and in some cases only one data point existed for a gas. There were several toxic gases that were not evaluated because only one non-zero data point was found, or no data points were found. Using this methodology, HBr, NH₃, and SO₂ were excluded for the LFP non-flaming scenarios, SO₂ and NH₃ were excluded for the NMC non-flaming scenarios, HCN and benzene were excluded for the LFP flaming

scenarios, and NH_3 was excluded for the NMC flaming scenarios. Some gases had limited data points with a wide variance, and in some cases these gases drove the results for exposure limit distances. For example, NO_2 and HCl produced the greatest AEGL exposure limit distances in the LFP non-flaming and NMC non-flaming scenarios, respectively. However, the NO_2 yield in the LFP non-flaming scenarios was calculated from data produced by a single study with % volume concentrations ranging from 1.3% to 9.7% [57]. The HCl yield in the NMC non-flaming scenarios was also calculated from data produced by the same one study [57] with % volume concentrations ranging from 0.2% to 9.7%. For vent gas temperatures, only four studies reported temperatures that had no contribution from flames. The average vent gas temperature was lower than expected, which may be due to the difficulty of measuring vent gas temperature. Regarding particulates, only four studies assessed metal particulates produced during thermal runaway. Assessments of particulate yields and size distribution only examined non-flaming conditions, therefore the models for flaming scenarios were required to use the data from non-flaming conditions. However, particulate yields and sizes are expected to vary significantly between flaming and nonflaming conditions. Additionally, data for particle composition from LFP thermal runaway was not found, so the inputs were extrapolated from the data available for NMC thermal runaway. These issues highlight the need for additional work to be done on characterizing toxic gas and particulate production during Li-ion thermal runaway (non-flaming and flaming).

The aggregated data used to develop inputs primarily came from cell or module level thermal runaway testing. The data was extrapolated to the unit level using energy capacity; however, more research is required to determine if this correlation remains accurate at the unit level. Additionally, BESS units contain other flammable materials aside from the Li-ion cells, i.e., electrical components. The contribution from these materials was not considered in the majority of reviewed studies as they were not relevant at the cell or module level. When selecting data for a specific BESS evaluation, it is imperative that the relevant stakeholder or user assess the characteristics and methodologies of the experimental studies to determine which are most appropriate. Additional analysis of the contributions to HRR and gas and particulate yields from these materials may be necessary.

All limitations identified in the dataset can cause uncertainty in the model. In the presented methodology, the average and positive standard deviation were calculated for gas and particulate yields where data was available, then added together to determine model inputs. The calculated standard deviations showed that there was significant variation in the results for all relevant parameters. To account for uncertainty in the experimental data, the upper bound of the dataset (average plus positive standard deviation) was utilized for model inputs. The lower bounds of the gas and particulate yields were not evaluated as the objective of the study's methodology was to assess the worst-case gas concentrations. Mouilleau & Champassith (2009) performed a validation for FDS modeling of atmospheric dispersion. They found that the outputs of the models fell within experimental uncertainty, except for under unstable atmospheric conditions or when wind was not modeled explicitly. In these cases, the FDS model overpredicted concentrations [115]. In the present study, wind was not modelled explicitly and therefore it can be assumed that the FDS model outputs predict the worst-case scenario for toxic gas dispersion without additional increases for uncertainty. When considering the results of the analysis performed by AERMOD, several studies of other dispersion events have found that AERMOD can overpredict or underpredict gas concentrations within a fractional bias of plus or minus two [116][117][118]. Additional model validation efforts, specifically for BESS thermal runaway gas dispersion events in both FDS and AERMOD would provide invaluable information on the uncertainties of the model predictions.

HF has been extensively studied, and while additional research on HF production from Li-ion cells would be useful, attention to other gases including HBr, HCl, NO₂, SO₂, HCN, NH₃, and benzene is essential for future comprehensive evaluations of health and environmental impacts. Similarly, there was a lack of data regarding particulate composition, size distribution, and yield. In total, seven studies evaluated particulate; however, three studies were excluded as they did not report data necessary for particulate deposition modeling or did not report the sampling method. Additionally, there were no studies identified that reported usable particulate yields or sizes for flaming thermal runaway incidents, in which particulate characteristics are expected to be significantly different due the effects of combustion. Furthermore, there was only one study that looked at particulate yield and size distribution for LFP cell chemistry. Data on particulate composition for LFP cell chemistry was not available so the model inputs had to be extrapolated from data for NMC cell chemistry. To properly characterize particulate emissions from Li-ion thermal runaway, further research is required, especially for flaming conditions.

The relationship between molecular weight and concentrations under lower gas production rates should also be further explored. Plumes with higher mass release rates were more buoyant and less likely to have variation in the exposure limit distance by species. However, there were different trends in the impact of wind speed, ambient temperature, and incident duration for different toxic gas species for the LFP non-flaming scenario at a 12-hour incident duration. FDS utilizes molecular weight as a factor in gas dispersion, therefore it is likely that the influence of this property on plume dispersion became more visible when the plume was less concentrated and less governed by buoyancy due to temperature and velocity, e.g., LFP, non-flaming, 12-hour scenario.

In the non-flaming scenarios, AERMOD model results tended to produce shorter community exposure limit distances than FDS, while in the flaming scenarios, FDS tended to produce shorter community exposure limit distances. For example, for LFP-non-flaming scenarios, the maximum distance to reach AEGL-1 concentrations for HF was 168 m in FDS compared to 61 m in AERMOD. For LFP flaming scenarios, the maximum distance to reach AEGL-1 concentrations for HF was 16 m in FDS compared to 83 m in AERMOD. The reason for the discrepancies between the two models is likely a result of the intended uses for each model and its associated limitations. FDS utilizes CFD which accounts for flow velocities and turbulence to model plumes generated from fuel combustion. AERMOD on the other hand was created to model dispersion of plumes from industry processes and utilizes gaussian theory which employs simplified flows that are not dominated by buoyancy. The methodology utilized in this study for the flaming scenario models in AERMOD attempted to capture the characteristics of the plume post-combustion, however, the plume area utilized did not capture the full volume of air being entrained into the plume and subsequently traveling within it. Additionally, the FDS results showed that the velocity in the centerline of the plume continued to increase at heights above where combustion ceased. As such, the buoyancy and density of the plume in AERMOD were not as high as modeled in FDS. Further, the AERMOD point source was set at a height equal to the top of the BESS unit, not where the measurements for the temperature and velocity inputs were taken. This was done because the measurements were taken in a no-wind condition scenario in FDS, but it was expected that high winds would drive this height down, and thus this was a conservative assumption. Because the release point was lower in AERMOD, the plume was closer to the ground, causing higher breathing height concentrations.

While AERMOD may be capable of high-level predictions of long-range plume dispersion and grounding, FDS is likely more suitable for near-field analysis (up to 200 m) in scenarios involving combustion. In a comparison between the capability of FDS and SCICHEM, a Lagrangian plume dispersion model, to simulate plume dispersion from a BESS thermal incident, EPRI found that FDS predicted 2-3 times higher centerline concentrations of gases over distances 0-250 m downwind and a smaller horizontal plume width [119]. EPRI attributed this difference to atmospheric turbulence which is not accounted for in FDS [119]. The same is likely the case in this study, where less atmospheric turbulence in FDS allows the plume to remain more concentrated as it travels horizontally. This effect is more pronounced in the non-flaming scenarios where less turbulence occurs due to the lack of air entrainment caused by combustion; the plume remains closer to the ground because of lower plume temperatures and less buoyancy. This suggests that atmospheric models that account for turbulence in the atmosphere, such as AERMOD, in conjunction with real-world meteorological data, are better suited for plumes produced from non-flaming thermal runaway conditions, especially in the far-field. Further research on the most suitable plume dispersion model for different thermal runaway conditions, e.g., flaming versus non-flaming, would provide beneficial insight for engineers.

The results produced by this methodology are specific to the baseline scenario created for the purposes of this study. To apply this process to a specific unit, the relevant stakeholder or user must conduct an analysis of the specific BESS unit, relevant thermal runaway data, surrounding environment, and location of nearby communities. When choosing thermal runaway data, all data points found in Section 3.1 were considered to characterize the gas production rate and heat release rate. However, for analyzing a specific BESS, the data that is not relevant to the BESS unit should be excluded. The environmental impact guidelines that were utilized in the baseline scenario of this study are focused on freshwater organisms and earthworms. LC₅₀ and EC₅₀ values are available for saltwater/marine organisms and other land-dwelling organisms, as well as for predators and organisms that live in the sediment in water. The modeled environment and chosen guidelines are specific to the baseline scenario based on Lemoore, CA. For a project-specific hazard assessment, it is necessary to characterize the location of the BESS unit before choosing the guidelines and relevant location(s) for ecotoxicological evaluation.

6. Summary

This research presents a methodology to assess the health and environmental impacts from thermal runaway events in outdoor, large-scale, Li-ion BESS units. Through application of the methodology, a relationship between exposure limit distance and wind speed, ambient temperature, event duration, cell chemistry, and toxic gas species can be established.

A literature review was conducted to aggregate available data on Li-ion thermal runaway, historical Li-ion BESS incidents, and Li-ion thermal runaway modeling practices. The literature review revealed variations in thermal runaway test methods. Studies had different methods for thermal runaway initiation, type and arrangement of the cells, and HRR, THR, MLR, and gas characterization and quantification. Additionally, the definition of thermal runaway varied between researchers with different temperature ranges or measurements being suggested to define thermal runaway. The variation in approaches presents challenges when comparing data sets. While UL 9540A provides a standardized testing method, there is no requirement for quantification of the full range of gases produced during thermal runaway; the focus is not toxic gases, it is gases that can cause an explosion. As such, data sets from UL 9540a tests, while more

easily comparable, are limited in scope. A review of actual incidents revealed that, oftentimes, the unit model and specifications are not made publicly available so details on cell chemistry, type, and arrangement are lacking.

Using the HRR and heat of combustion, the MLR can be calculated for a combusting fuel. Non-flaming thermal runaway does not produce a flame, therefore, use of HRR and heat of combustion to predict MLR would not be appropriate. Instead, the MLR was determined by dividing total estimated gas production by event duration. The flaming thermal runaway was characterized by dividing THR by event duration. Total gas production and THR were found by taking the average total gas production or THR normalized by capacity and multiplying by the capacity modeled in each scenario. The worst-case amount of fuel consumed for the non-flaming scenario was one bay or 0.49 MWh due to heat transfer being restricted and unlikely to initiate thermal runaway in other bays. The worst-case amount of fuel consumed for the flaming scenario was the full BESS unit or 3.101 MWh based on historical incidents. Duration for the non-flaming cases was based on cell venting times. Incident duration for the flaming cases was based on historical incidents. This provided an average MLR or total gas production rate for each scenario that was applied to gas emission yields to find species production rates. Typically, yields were quantified in mass produced normalized by mass consumed or percent volume composition. Sometimes, they were also quantified in mass produced normalized by capacity. The methodology prioritized mass produced normalized by mass consumed and percent volume composition, because they could be directly applied to the average MLR and are unlikely to over- or underestimate the mass loss. HF was identified as the most unique hazard of Li-ion BESS thermal runaway events, based on the literature review.

Near-field health impact was analyzed via the FDS simulation results. Far-field health impact and environmental impact were analyzed via the AERMOD simulation results. Models were run with a bounding wind and temperature analysis in FDS only. Due to AERMOD's reliance on real-world weather readings, an analysis on a range of prescriptive meteorological conditions could not be performed. Instead, a baseline scenario was constructed using weather data for Lemoore, CA. Both FDS and AERMOD utilized the same emission rate inputs. Human health impact was evaluated by measuring the distance at which occupational or community exposure limits for gases were exceeded, i.e., IDLH and PAC, respectively. This study did not consider other health factors, such as thermal exposure. Environmental impact was evaluated by determining the relevant LC₅₀ and EC₅₀ values based on the location, as well as the reference depth for soil and water. Deposition at a point of interest was calculated to provide an example of the environmental impact methodology.

When evaluating human health impact in the near-field in FDS, NO₂ produced the furthest distances for the LFP non-flaming scenarios for both occupational and community health impact exposure limits. HCl produced the furthest distances for the NMC non-flaming scenarios for both occupational and community exposure limits. HF produced the furthest exposure limit distances for the LFP flaming scenarios for both occupational and community exposure, as well as for the NMC scenario for occupational exposure. SO₂ produced the furthest distances for the NMC flaming scenarios for community exposure limits. Results from AERMOD showed the same species produced the furthest exposure limit distances.

Based on the FDS results, the non-flaming cases produce further exposure limit distances compared to the flaming thermal runaway cases due to the less buoyant plume remaining at breathing height. In FDS, the non-flaming scenarios have occupational exposure limit distances of

70 m and 81 m for LFP cells and NMC cells, respectively. These distances are the same order of magnitude as the 91 m safety distance recommended by the International Association of Fire Chiefs (IAFC) for large commercial systems [120]. The non-flaming scenarios have community exposure limit distances of over 200 m for both LFP cells and NMC cells. For the non-flaming cases evaluated in FDS, cell chemistry, wind speed, duration, and temperature had significant impact on exposure limit distances. In some cases, the type of toxic gas also influenced trends. The LFP flaming cases have distances of 1.125 m for occupational exposure and 16 m for community exposure. The NMC flaming cases have distances of 1 m for occupational exposure and 15 m for community exposure. For the flaming cases evaluated in FDS, wind speed was the controlling factor, with duration having some influence on exposure limit distances. Table 35 presents the FDS maximum exposure limit distances and conditions at which the exposure limit distances were reached.

Table 35. FDS exposure limit distances and critical species.

Thermal Runaway Conditions	Chemistry	Criteria	Wind [m/s]	Temp [C]	Duration [hr]	Gas	Distance [m]
Non-Flaming	LFP	IDLH	2	35	6	NO ₂	70
		AEGL	All	All	All	NO ₂	>200
	NMC	IDLH	10	22	0.5	HCl	81
		AEGL	5 & 10	All	All	HCl	>200
Flaming	LFP	IDLH	10	22 & 35	2	HF	1
		AEGL	10	22	4	HF	16
	NMC	IDLH	10	All	2	HF	1
		AEGL	10	35	6	SO ₂	15

Results from AERMOD show that the LFP non-flaming cases have an exposure limit distance of 322 m for community exposure. The NMC non-flaming cases have an exposure limit distance of 418 m for community exposure. The LFP flaming cases have an exposure limit distance of 83 m for community exposure. The NMC flaming cases have an exposure limit distance of 62 m for community exposure. Table 36 presents the AERMOD exposure limit distances and conditions at which the exposure limit distances were reached.

Table 36. AERMOD exposure limit distances and critical species.

Thermal Runaway Conditions	Chemistry	Duration [hr]	Critical Species	Distance [m]
Non-Flaming	LFP	6	NO ₂	322
	NMC	0.5	HCl	418
Flaming	LFP	4	HF	83
	NMC	4	SO ₂	62

In the non-flaming scenarios, AERMOD model results tended to produce shorter community exposure limit distances than FDS, while in the flaming scenarios, FDS tended to produce shorter community exposure limit distances. While AERMOD may be capable of high-level predictions of long-range plume dispersion and grounding, FDS is likely more suitable for near-field analysis (up to 200 m) in scenarios involving combustion (and buoyancy driven flow). Conversely,

atmospheric models that account for turbulence in the atmosphere (but not in the plume), such as AERMOD, in conjunction with real-world meteorological data, are likely better suited for plumes produced from non-flaming thermal runaway conditions, especially in the far-field. Utilizing this methodology, the overall single worst-case community exposure limit distances for the modelled LFP and NMC scenarios would be 322 m and 418 m, respectively, which were achieved during non-flaming conditions. The overall single worst-case occupational exposure limit distances for the modelled LFP and NMC scenarios would be 70 m and 81 m, respectively, which were also achieved during non-flaming conditions.

For environmental impact, concentrations that could exceed the LC_{50} or EC_{50} values for earthworms or aquatic organisms in the NMC non-flaming scenario were confined to the immediate vicinity of the BESS unit or within 60 m of the BESS unit. The results of the analysis on contaminated fire water runoff show that significant environmental impacts are not expected as the result of contamination with metals, fluoride, or chloride. While levels of these elements will be elevated, they are not high enough, due to the large quantities of water that are expected to be applied, to cause significant acute health impacts to water-based organisms.

The study findings related to exposure distances are specific to the modeled hazard scenarios and associated inputs; the relevant stakeholder or user should not apply the findings from this research in a site-specific hazard analysis without verifying that the modeled scenarios (and associated inputs) are applicable.

7. Appendices

7.1. *Summary of Peer Reviewed Studies*

7.1.1. [Amano et al., 2022](#)

Amano et al. (2022) performed 19 tests of NMC Li-ion battery cells in order to quantify the combustible and toxic gases produced during thermal runaway. The tests utilized NMC pouch cells with a 10 Ah/37 Wh capacity and a mass of 178 g and NMC pouch cells with a 32 Ah/118 Wh capacity and a mass of 590 g. Tests were of single cells or cell arrays consisting of two cells. Two series of tests were conducted. In Test Series 1, thermal runaway was initiated via a glow plug, and in Test Series 2, thermal runaway was initiated via a heating plate.

All tests were conducted in a 100 L sealed chamber, with ambient air. The SOC of the cell(s) varied between tests. Temperature and pressure measurements inside the chamber were used to determine the total amount of gas released from the cells. Gas samples were obtained from the chamber after the test was complete and were analyzed via FTIR. A thermal runaway onset temperature was defined as the temperature at which an obvious exothermic effect could be measured. A reaction temperature was defined as the maximum temperature achieved at the cell surfaces during the test. Using the time difference between these two temperature parameters, an effective period of thermal runaway was determined. The authors did not determine if flaming conditions were achieved for each test. The authors determined the average concentrations of the measured toxic vent gases for both test series; where multiple tests are grouped together, the average value across the tests is indicated.

The total gas production was observed to increase with increasing SOC. The authors noted that the tests involving one 10 Ah cell and two 10 Ah cells at 90-100% SOC had similar normalized gas production volumes despite the increase in cell capacity. They noted that this may have been due to the oxygen limited environment. HF was not detected in Test Series 2, however the authors noted that this may have been due to the increased dilution factor used in Test Series 2 (1:100) compared to that used in Test Series 1 (1:10). CO concentrations were observed to increase with increasing cell SOC and increased capacity. CO₂ measurements were not reported due to strong interference with other compounds [121].

7.1.2. [Amano et al., 2023](#)

Amano et al. (2023) performed 31 tests of NMC Li-ion battery cells in order to quantify the combustible and toxic gases produced during thermal runaway. Three series of tests were conducted. Test Series 1 utilized NMC pouch cells with a 2.5 Ah/9.25 Wh capacity and a mass of 58 g. Test Series 2 utilized NMC pouch cells with a 10 Ah/37 Wh capacity and a mass of 178 g, as well as NMC pouch cells with a 32 Ah/118 Wh capacity and a mass of 590 g. Tests were of single cells or arrays of two cells.

All tests were conducted in a sealed chamber, with ambient air. The chamber for Test Series 1 had a volume of 10 L, the chamber for Test Series 2 had a volume of 100 L, and the chamber for Test Series 3 had a volume of 45 L. The SOC of the cell(s) varied between tests for Test Series 1, while all cells in Test Series 2 were charged to 100% SOC. Test Series 1 and 2 initiated thermal runaway via heating plates. Test Series 3 initiated thermal runaway via overcharging. Temperature

and pressure measurements inside the chamber were used to determine the total amount of gas released from the cells. Gas samples were obtained from the chamber every 10 seconds and analyzed via FTIR.

For cells at a SOC of 50% or less, the authors determined that ignition of the vent gases did not occur. The publication did not indicate if ignition occurred during the 80 and 100% SOC tests in Test Series 1. Ignition of vent gases was determined for most Test Series 2 tests. The authors reported the average concentrations of the measured toxic vent gases for Test Series 1 and 2; where multiple tests are grouped together, the average value across the tests is indicated. Gas concentrations for Test Series 3 were not reported.

A trend in HF production in relation to cell SOC could not be identified, but it was observed the highest average concentration (18 ppm) was produced during tests of cells at 100% SOC. HF was not detected in Test Series 2, however the authors noted that this may have been due to increased dilution because of the increased size of the test reactor (100 L) compared to that used in Test Series 1 (10 L). HCN concentrations were observed to increase with increasing cell SOC [62].

7.1.3. Archibald 2021

In this dissertation from the University of Texas at Austin, Archibald conducted a series of experiments with single Li-ion cells, as well as cell arrays and modules to determine gas release and thermal runaway propagation behavior.

The first series of single-cell experiments were conducted using LCO pouch cells with a 5 Ah/18.5 Wh capacity at 100% SOC. The cells each had a mass of 90.2 g. Two tests were conducted in open air, and one was conducted with an inert pressure vessel. The cells were externally heated with block heaters on either side of the cell. The tests showed that the cells began to slowly vent approximately 1000 seconds before the rapid heating associated with the onset of thermal runaway. The author estimated that approximately 15% of the total vent gas was released during this incipient period. Thermal runaway was initiated when the heater-cell interface temperature reached 185 to 196°C. During the test, temperatures as high as 900°C were measured close to an emerging hot gas jet.

Cell array experiments were conducted with the same LCO pouch cells utilized in the single-cell experiments described above, as well as with 10 Ah LCO pouch cells. The 10 Ah cells had a mass of 208.9 g. Tests included either 5-cell arrays or 10-cell arrays, with the cells clamped together linearly with no insulation or spacing between them. A cartridge heater was utilized to initiate localized heating at the center of the initiating cell. The arrays were contained in a pressure vessel purged with nitrogen.

For the 5 Ah arrays, the tests showed that the average time for cell venting was 11 seconds, and the average time for thermal runaway propagation between cells was 15 seconds. Upper gas temperatures in the chamber reached a maximum of approximately 150°C in the 10-cell, 5 Ah array test and approximately 130°C in the 10-cell, 5 Ah array test. For the 10 Ah arrays, the tests showed that the average time for cell venting was 14 seconds, and the average time for thermal runaway propagation between cells was 22 seconds. The author attributed the longer vent and propagation times to the increased thickness of the 10 Ah cells compared to the 5 Ah cells. Upper gas temperatures in the chamber reached a maximum of approximately 200°C in the 10-cell, 10

Ah array test. Archibald (2021) found that the final pressures and upper gas temperatures in the 10-cell, 5 Ah array and the 5-cell, 10 Ah array were nearly identical, and thus, concluded that the volume of vent gases and heat release can generally be normalized by watt hour capacity; additional testing was recommended to confirm the trend.

In comparing the single-cell tests to the cell array tests, it was found that single cells experience a longer pre-heat period, and the period of intense venting is faster than a cell that achieves thermal runaway via cell-to-cell propagation. The single cells also vented gas during the pre-heat period before thermal runaway. Conversely, the cells in the array did not have time to vent gases, because the preheat period lasted only a few seconds.

In the second series of single-cell experiments, tests were performed in a burn structure and in a pressure vessel purged with nitrogen. The cells used were NMC prismatic cells with a nominal capacity of 94 Ah/346 Wh and a nominal voltage of 3.68V. Cells were at 100% SOC and had a mass of 2100 g. Three single-cell, open air tests were conducted in the burn structure. In the first test, the cell was heated with a cartridge heater. This method caused the cell to rupture and project across the room, compromising the usefulness of the collected data. The next two tests utilized electric heaters on the large face of the cell with a gradual heating rate of 5°C/min. In these two experiments, the cell vent opened and started to release gas 368 seconds and 292 seconds prior to thermal runaway and intense venting. The temperature of the gas measured immediately above the vent reached a maximum of 750°C during the intense venting period. The cell had a total mass of approximately 1350 g at the end of the test (750 g mass loss).

One single-cell, NMC test was conducted in the inert pressure vessel. The test utilized an electric heater on the large face of the cell, with a gradual heating rate of 5°C/min. Measured gas temperature and pressure were used to calculate the total volume of gas released from the cell and the gas release rate. The total volume of gas released was found to be 221.6 L at STP. The authors normalized this gas volume by cell energy capacity with a calculated value of 0.64 L/Wh. The total venting time was 7 seconds, and the peak gas release rate was calculated to be approximately 65 L/s. The composition of the vent gas was determined via a gas chromatography thermal conductivity detector (GC-TCD) calibrated to measure calibrated to measure H₂, N₂, CO, methane, acetylene, ethylene, ethane, propylene/propane, and water. Archibald (2021) reported the percent volume composition of the vent gases produced by the single NMC cell, with the majority of the gases being made up of H₂, CO, and CO₂.

Archibald (2021) also conducted several module level experiments comprised of the same 94 Ah, NMC cells used in the single-cell tests described above. The module consisted of fourteen cells, connected in series, within a polycarbonate casing. Thermal runaway was initiated via the same electric heater method used in the single-cell experiments. One module test was conducted in open air and two were conducted inside a steel rack enclosure to represent a BESS installation. The steel enclosure was closed on all sides, including the top side, with vent openings only at the top and bottom of the front side. Two noncombustible “dummy” models were installed above the test module within the enclosure.

In the open-air module experiment, a single cell was forced into thermal runaway and propagation subsequently occurred throughout the remaining cells. The authors observed that the failure of cells was generally similar to that observed in the single-cell tests. The initiating cell began to vent, and 77 seconds later, intense venting occurred, ejecting flammable gas and other materials from the cell over a period of several seconds. The flammable gases ignited during this

intense venting period. Similar behavior was seen throughout the experiment for each cell as it failed via propagation. Propagation time for the first five cells was on the order of magnitude of minutes; however, as the event progressed, cell-to-cell propagation time decreased so that propagation through the last nine cells occurred over a total time of approximately 250 seconds, or approximately 27 seconds per cell. The total duration from thermal runaway of the initiating cell to completion of thermal runaway of the last cell was approximately 17 minutes. Mass loss measurements indicated that at each intense cell venting event, there was an approximate mass loss of 900 g. Using a time of 5 seconds before thermal runaway and 15 seconds after, the authors calculated an estimated average MLR of up to approximately 45 g/s during a single cell vent event and up to approximately 55 g/s over the period of time at which two cells vented in rapid succession. Between cell venting events, gradual mass losses occurred due to combustion of the module's polycarbonate housing. The total cell mass loss during the test was estimated to be approximately 12,200 g and the total mass loss of the polycarbonate housing was estimated to be approximately 3,000 g. Gas temperatures within the module reached a maximum of approximately 1180°C.

In the rack module experiments, similar behavior was seen for thermal runaway propagation. The total duration from thermal runaway of the initiating cell to completion of thermal runaway of the last cell was approximately 16.5 minutes, compared to 17 minutes in the open-air test. For all three module experiments, the last 3 cells underwent thermal runaway in a period of 20 to 38 seconds. Gas temperatures within the module and within the rack enclosure reached a maximum of approximately 950°C.

Archibald (2021) also performed a series of tests to evaluate the explosion hazards of Li-ion cells. As part of this series, a test of an array of five, 18.5 Ah, LCO pouch cells in an inert pressure vessel was conducted. This test produced a total of 118.2 L of gas, or 0.35 L/Wh. Archibald (2021) reported the percent volume composition of the vent gases produced by the 5-cell array, with the majority of the gases being made up of H₂, CO, and CO₂.

In a review of 21 studies on gas compositions of Li-ion cell venting incidents at 100% SOC, Archibald found that gas released per nominal capacity was a minimum of 0.12 L/Wh, a maximum of 0.63 L/Wh, and an average of 0.40 L/Wh, across various cell chemistries.

Additional experiments were conducted on modules comprised of cylindrical, Type 26650, LFP cells. The module contained 48 cells arranged with six cells long, four cells wide, and two cells high. The two vertical rows of cells were separated by a thin plastic panel and thin foil current collectors. The module had a total nominal capacity of 568.3 Wh (11.8 Wh per cell) and a total mass of 5300 g.

The first experiment was conducted with the module in open-air. Thermal runaway was initiated via a block heater placed under 12 of the bottom cells. These 12 cells were observed to enter thermal runaway within 918 seconds after the first cell vent. Propagation to other cells in the module did not occur for another 305 seconds. The next 14 cells went into thermal runaway over a period of 813 seconds. Analysis of mass loss rates showed that individual cell vent events had an average MLR of 1 g/s to 3 g/s. The cells that experienced higher MLR were determined to be those that partially ejected their contents (i.e., cathode, anode, current collectors). The total mass of the module at the end of the test was approximately 4965 g (335 g total mass loss). No flaming conditions were achieved during the test and post-test evaluation showed that only the 24 lower

cells went into thermal runaway. As such, thermal runaway was noted to have propagated horizontally within the module, but not vertically.

The second experiment consisted of only the bottom 24 cells of the module, located within a pressure vessel purged with nitrogen. Thermal runaway propagated throughout the 24-cell array over a period of 909 seconds. The event produced a total of 33.5 L of gas at STP, or 0.12 L/Wh. The total starting mass of the array was 2,080 g and the total mass at the end of the test was 1,566 g (514 g total mass loss). Upper gas temperatures within the chamber reached a maximum of approximately 190°C. Archibald (2021) reported the percent volume composition of the vent gases produced by the single NMC cell, with the majority of the gases being made up of H₂ and CO. Comparing the tests involving LMC and LCO cells and those involving LFP cells, Archibald (2021) observed that the LFP tests did not achieve flaming conditions due to the lack of ejected hot material. In the LCO and NMC tests, the cells consistently ejected glowing hot particles, which almost immediately ignited the surrounding gases [56].

7.1.4. Andersson et al., 2013

The SP Technical Research Institute of Sweden performed experimental testing on Li-ion battery electrolytes to assess the production of HF, PF₅, and POF₃ and the feasibility of using FTIR to measure the gases. In addition, the authors initiated flaming thermal runaway in pouch and cylindrical Li-ion cells, as well as two laptop battery packs, to quantify thermal combustion characteristics method under different heating and combustion conditions. The FTIR spectrometer was a Thermos Scientific Antaris IGS analyzer.

In the first phase of the study, two types of tests were run under a cone calorimeter. The first involved placing the electrolyte materials in an open container and heating them via external radiation. The second type was an extension to these tests where the vapor produced from the thermal decomposition of the electrolyte materials was ignited via an electric sparker. The FTIR sampling port in the exhaust duct was located approximately 20 inches upstream of the radiant cone. Independent tests were run with different combinations of electrolyte materials and mixtures. LiPF₆ salt and two types of solvents, dimethoxyethane (DME) and propylene carbonate (PC), were used in this phase. It was found that evaporation of pure LiPF₆ salt and combustion of LiPF₆ salt dissolved in both types of solvents produced HF and POF₃ but did not produce PF₅.

The second phase of the study involved tests that injected solvent/salt solutions directly into a propane burner flame. The burner effluents were collected under the cone calorimeter hood, and it is assumed that the FTIR sampling port was in the same location as previous tests. Variations of the test were conducted with different propane/solvent ratios, salt/solvent concentrations, and introduction methods of the solution into the flame. In addition, some tests involved injecting water into the flame as well. The two types of solvents used in this phase were DME and DMC and the salt was LiPF₆. It was observed that HF and POF₃ were always present during the combustion of the electrolyte solutions. The HF concentration was 8 to 33 times higher than the POF₃ concentration in each of the tests involving DMC and 53 times higher in the one test involving DME. No reasoning for the difference in the HF/POF₃ ratio was established. Peak concentrations of HF reached as high as 1,500 ppm and peak concentrations of POF₃ reached as high as 158 ppm in the exhaust duct, i.e., close to the source. In addition, no conclusive findings were identified for the impact of water on HF or POF₃ production. PF₅ was not detected in any of the tests. Andersson et al. (2016) identified that the Swedish Work Environment Authority set a maximum allowable

concentration of HF in a working environment at 2 ppm and the NIOSH sets the IDLH value of HF at 30 ppm but neither of these organizations have established exposure limits for POF_3 .

The gas sampling system included a pump to draw in sample gas, filters, and a gas cell. The pouch cells tested were placed in five cell bundles and fastened together with steel wire. The cylindrical cells were placed in a bundle of nine cells and placed in a box made of steel net and silica board. The two laptop battery packs were placed inside a steel net. The experiment was conducted in an SBI apparatus, and a propane burner was utilized to initiate combustion. HRR was measured via oxygen consumption calorimetry. Water mist was applied to Test 3 only. The authors report the test specifications and results for mass loss, heat release, and toxic gas production. At the higher SOC, pouch cells underwent rapid venting of gases, whereas no rapid venting was observed in the lower SOC pouch cell tests. The rapid venting of gases was also observed in the cylindrical cell and laptop battery pack tests. Andersson et al. (2013) noted that the water mist applied in Test 3 did not impact the total amount of HF produced, although it had the potential to shift the chemical kinetics to favor HF production over POF_3 [18].

7.1.5. Barone et al. 2021

Barone et al. (2021) assessed the morphology and elemental composition of Li-ion thermal runaway particulates by forcing battery cells at 100% SOC into thermal runaway, via the EV+ ARC. The cells were cylindrical, spiral-wound, with LiFP_6 electrolyte, and NMC, LTO, and LFP chemistries at capacities of 3.2 Ah, 3.8 Ah, and 1.3 Ah, respectively. After the cells vented, the heaters in the ARC were shut off. Aerosols were sampled on filters with a 200 nm pore size at a rate of 1 L/min for 5 seconds. The ARC apparatus mixes the aerosols before quantification, so the concentration of each element was not assessed. Composition was determined using SEM/EDS. Samples were sputter coated with gold and palladium. Lithium could not be measured with the type of SEM/EDS machine used in the study. Background aerosols were collected but were found to be negligible.

The NMC cell had a more intense and shorter vent duration in comparison to the LFP and LTO cells. During the test, the NMC cell ejected from the sample holder due to its violent explosion and produced embers, whereas the LFP and LTO cells did not eject, but emitted smoke continuously. More aerosols were emitted from the NMC cells than the LFP and LTO cells. The LTO cell produced less smoke compared to LFP and partially ejected its cell contents.

EDS mapping showed that NMC aerosols were either a) fragments of the anode/cathode, b) microspheres, or c) nanoparticles. For the NMC cells, anode/cathode fragments resembled the battery material and had a similar composition to the anode/cathode pre-incident (nickel, manganese, and cobalt). Particle sizes ranged from 5 to 10 μm , which the authors noted fell within the upper range for respirable aerosols. NMC microspheres contained nickel, aluminum, carbon, fluorine, and oxygen and had a size range of 0.1 to 3 μm . Barone et al. (2021) attributed carbon, fluorine, and oxygen to the LiFP_6 electrolyte solution. LFP aerosols were primarily cenospheres (hollow spheres) ranging from 0.6 to 5 μm . Cenospheres were composed of carbon, silicon, and fluorine, which the authors attributed to anode composition. No heavy metals were found. The LTO cell produced spheroids and cenospheres in the 0.1 to 4 μm range, as well as anode/cathode fragments containing cobalt and titanium [122].

7.1.6. Barowy et al., 2021

In 2020, UL conducted mock-up installation level BESS tests to assess the impact of water-based and clean agent fire suppression on installation level BESS fires. The tests involved an initiating unit, two partial target units, and several dummy units all placed in a 20-foot storage container. One target unit was placed directly next to the initiating unit, while the other was placed across from the initiating unit with separation. In the storage container, some walls were made of steel only, while other walls were a combination of steel, oriented strand board, and gypsum, or a combination of steel, polyurethane (PU), two layers of plywood, and gypsum. The container was equipped with five deflagration vents set to activate at 0.5 psig.

The initiating unit consisted of a rack of nine modules with a total capacity of 28.9 kWh. Each module contained 270, NCA, 18650, Li-ion cells at 100% SOC with a capacity of 99 Ah. The cell level thermal runaway properties are reported by the authors. The cells and modules were not electrically connected, meaning no current was running through them. The partial target units held one-third of the initiating unit's capacity, while the dummy units were empty. One cell in the initiating unit was heated to thermal runaway via film heaters. Tests were run without any suppression (Test 1), with Novec 1230 at 8.5 %vol (Test 2), and with water suppression (Test 3). Tests were terminated by discharging 41 kg of CO₂ into the container when thermal runaway activity subsided, or module temperatures began decreasing.

In Test 1, the initiating cell vented at 23 min 43 s and entered thermal runaway 2 min 22 s later. An off-gas plume was produced and ignited the initiating module 31 seconds after thermal runaway. There was a partial volume deflagration that opened the doors due to pressure, but the vents remained sealed. At this time, the combustible gas detector registered 50% of the lower explosive limit (LEL). The doors were manually closed and flaming subsided 1 min 25 s later. Thermal runaway propagated through all modules in the initiating unit and the left target within 2 hr 50 min of the initial thermal runaway. CO₂ was discharged 2 hr 55 min after thermal runaway initiation; no reignition occurred after CO₂ application.

The incident heat flux exceeded 12.5 kW/m², the critical heat flux for ignition of most combustible materials, at the rear wall after thermal runaway propagated to the modules and towards the end of the test and at the left target unit after the doors closed for the rest of the test. The rear and side walls had charring. There were penetrations to the bare steel beneath the plywood on the rear wall. The front target did not have as much exposure to heat flux, likely due to the separation distance.

The authors defined thermal runaway as “an immediate temperature increase of more than 400°C, and a sustained temperature above 300°C.” Thermal runaway propagated upward at a rate of one module per 2 to 10 minutes. Downward propagation was slower at a rate of one module per hour.

The gas concentrations were measured via portable gas detectors inside and outside the storage container for Test 1. Exterior sensors were located on Sides A and B of the container; both pumped, and diffusion sensors were used. The LEL peaked at 83% at 26 min into the initial thermal runaway event. At that point, thermal runaway started to propagate to the left target. The other gases peaked around 60 minutes into the test, except for the interior H₂, CO, and HCN which reached the measuring limit of the detectors shortly after thermal runaway. VOC concentrations also hit the measuring limit but dropped several times during the test. H₂S remained under 20 ppm both inside

and outside the container, but exterior measurements had higher readings than interior measurements. Gas concentrations tended to be higher on Side A, except for LEL.

Thermal runaway was first detected at 28 min 9 s for Test 2. The Novec 1230 system triggered after two smoke detectors were alarmed 55 seconds after thermal runaway. Thermal runaway propagation continued in the initiating module for 7 minutes after suppression. An upper layer of flammable gases formed and ignited 28 min 32 s after initial thermal runaway. The flames extinguished after 30 seconds, but the gas layer reformed and caused a deflagration 16 min later. The deflagration opened a side and ceiling vent. Thermal runaway propagation began again in Module 4 of the initiating unit. Thermal runaway reached the left target at 1 hr 1 min after the initial thermal runaway. Upward propagation continued at a rate of 1 to 12 minutes per module. At 2 hr 9 min, the door was opened, and a flashover occurred due to the introduction of fresh air. Water was applied manually to reduce the heat release rate, the doors were closed again, and the container was flooded with CO₂. Thermal runaway continued after CO₂ application. By the end of the test, all modules in the initiating unit and the left module had undergone thermal runaway.

The peak heat fluxes at the rear and side walls for Test 2 were comparable to Test 1 due to reignition after suppression. After the Novec 1230 was applied, the heat fluxes and temperatures inside the container decreased. There was a gradual increase after suppression that peaked at flashover. Temperature decreased after CO₂ was applied, but heat flux continued to slowly increase.

For Test 3, thermal runaway initially occurred at 29 min 53 s. After 8 min 49 s, thermal runaway had propagated throughout the initiating module. Ignition and sustained flaming occurred at the same time. The water suppression system turned on 10 min 13 s after the initial thermal runaway. Flaming was suppressed, but cooling the module was not as effective due to the initiating unit's enclosure protecting the modules from direct contact. As a result, partial thermal runaway occurred in three more modules in the initiating unit. Deflagration occurred when the third module went into thermal runaway. Waterflow was stopped 1 hr 36 min into the test. Two more modules in the initiating unit underwent thermal runaway. Eventually, thermal runaway propagated to the left target. Waterflow was turned back on to see if cooling would prevent further propagation. At 2 hr 29 min, the storage container doors were opened while maintaining suppression. One module at the top of the initiating unit entered thermal runaway.

The temperatures at the rear and sidewall peaked at ignition and were lowered during suppression. After suppression was turned off, both temperature and heat flux increased and peaked once more. The temperatures inside the target units followed a similar pattern. In total, seven modules from the initiating unit and one module from the left target underwent thermal runaway.

The Novec 1230 at 8.5 %vol did not remove sufficient heat to stop thermal runaway concentration. Other studies demonstrated that propagation could be reduced using crossflow at the same concentration but did not completely stop it [123]. Tests 1 and 2 had the same extent of thermal runaway propagation and similar rates of propagation. The Novec 1230 only delayed initial propagation from the initiating module. The water suppression in Test 3 lowered the temperatures enough to reduce thermal propagation but did not eliminate it. The modules in Test 1 and Test 2 reached the same magnitude of temperatures, although there was a delay in Test 2. The suppression in Test 3 consistently lowered temperatures when active, but the temperatures would increase after the waterflow was discontinued. Deflagrations occurred in all three tests and

were associated with the thermal runaway of a module. It is possible that the gases were ignited due to hot surfaces or sparks caused by thermal runaway, or the electrically powered gas detectors inside the enclosure. However, the vents mitigated the severity of deflagrations. Test 3 saw lower gas concentrations compared to Tests 1 and 2 due to less thermal runaway propagation, but neither suppression system stopped flammable gas accumulation. All three tests reached the upper flammability limit and greatly reduced oxygen (7 to 10 %vol). CO was measured at 2 to 3 times higher yields than under-ventilated compartment tests containing plastics or PU foam. CO₂ was measured at 2 to 4 times higher than IDLH.

Novec 1230 was insufficient for cooling, but water suppression may be useful for mitigating thermal runaway between units. However, the module-to-module propagation was not affected by suppression. Gas temperature increase can raise the thermal propagation rate exponentially. Separation between units could stop thermal propagation due to less exposure to high temperatures. Thermal runaway is more likely to propagate upwards than downwards, and an event where the bottom module initiates thermal runaway may be more hazardous [53].

7.1.7. Bergstrom, 2015

In this study, tests in an inert environment were conducted for thermal runaway of LFP and NMC pouch cell batteries to assess the gases and metal particulates released during the events. All tests were on a single cell. The energy capacity of the cells was not provided in the publication. For each test, the cell was placed inside a small steel box, referred to as a “battery box”, that was purged with humidified nitrogen (63% relative humidity). The battery box was placed inside a glove box which served as the test chamber and the sample location for ventilated gases and aerosols. Gas sampling of semi-volatile and volatile compounds was performed with adsorbent tubes (Tenax and Carbosieve) and TD-GCMS was utilized for gas analysis. Additionally, FTIR was used for gases not expected to be adsorbed by the Carbosieve tubes, particularly HF and CO. Particulates were collected via polyvinyl chloride (PVC) and glass fiber filters and metals were analyzed via ICP-MS.

Thermal runaway was initiated via an electric heating element on the underside of the battery box. The heater was active until visual signs of aerosol release from the battery box were observed. Upon this observation, sampling was started and continued for a duration of 10 minutes. Temperatures inside the battery box reached a maximum of approximately 155°C in the LFP cell tests and 225°C in the NMC cell tests.

For both cell chemistries, the most prevalent semi-volatile and volatile gases were carbonates, with DEC (1 ppm) and ethyl methyl carbonate (EMC) (1 ppm) identified in the LFP cell tests and DMC (0.3 ppm) and EMC (1 ppm) identified in the NMC cell tests. Phosphorofluoridates were only identified in the NMC cell tests. Hydrogen fluoride was only detected in LFP Test 1, which was the only test for which the gas samples did not have to be diluted. The maximum detected HF concentration in LFP Test 1 was 50 ppm. Drager tubes were also utilized and across all tests, these showed that HF levels were highest in the early stages of cell ventilation. The highest HF concentration measured via the Drager tubes was greater than 200 ppm in an NMC cell test. The FTIR sampling did not detect CO in any of the tests.

The mass loss of the cells in each test were 30 g, 43 g, 49 g, and 46 g, for LFP Test 1, LFP Test 2, NMC Test 1 and NMC Test 2, respectively. The maximum detected metal concentrations and total suspended particles for the two cell chemistries were reported. The authors noted that the

lithium levels in LFP Test 2 were above the ceiling limit value of 0.02 ppm established by the Swedish Work Environment Authority [124].

7.1.8. Blum & Long, 2016

In cooperation with the Fire Protection Research Foundation (FPRF), Exponent, Inc. conducted a hazard assessment of Li-ion BESS. The analysis included full-scale fire testing of Tesla Powerpacks at the Tesla test facility in November of 2015. A PowerPack consists of approximately 14,400 cylindrical, 18650 cells, each with a nominal voltage of 3.6V and a capacity of 2.4 Ah. The total capacity of a PowerPack is 100 kWh. Cell chemistry was not indicated in the report, but it is understood that the PowerPack utilizes NMC cells.

The analysis included a literature review which identified that Li-ion battery cells, when subjected to abnormal heating, can vent vaporized electrolyte products and electrolyte decomposition products. The gases released depend on cell composition, SOC, and the cause of cell venting and can include VOC (such as alkyl-carbonates, methane, ethylene, and ethane), H_2 , CO_2 , CO, soot, and particulates containing oxides of nickel, aluminum, lithium, copper, and cobalt. The literature review also found that during fires involving Li-ion batteries, NO_x , HCN, and HCl can be produced, and concentrations of fluoride and chloride may be found in water samples collected after extinguishing such fires. These findings of the literature review were applicable to Li-ion batteries generally, not specifically Tesla equipment.

Full-scale testing of the Powerpack was conducted in two configurations, an internal ignition test and an external ignition test. The internal ignition test was performed by placing cartridge heaters in the center of a pod module, and the external ignition test utilized a propane burner to generate direct flame impingement on the exterior side of the unit. Both tests used 100 kWh Powerpack units at a 100% SOC. Products of combustion were measured via handheld gas sampling units with built-in pumps which drew air samples from the exhaust vent of the unit. The following gases were measured: CO, Cl_2 , CH_4 , and HF. Heat flux measurements were taken during the test, however the results were deemed to be inaccurate, and therefore, were not considered in the findings of the hazard assessment.

For the Internal Ignition test, there was no flaming, only white smoke. Thermal runaway did not propagate beyond the initiating energy pod. The test duration from first smoke to extinguishment was 75 minutes. CO concentrations reached the maximum detectable limit of the sensor (2000 ppm) for 51 minutes. Cl_2 was not detected. CH_4 reached a maximum volume fraction of 96.9% vol. HF reached a maximum concentration of 26 ppm for 2 minutes and then steadily decreased.

For the External Ignition test, there was sustained flaming for 176 minutes. Thermal runaway propagated to all energy pods. CO concentrations reached a maximum of 50 ppm while external burners were on, but CO was not detected after the burners were turned off. Cl_2 and CH_4 were not detected. HF reached the maximum detectable limit of the sensor (100 ppm) for the last 30 minutes of the test.

The HF concentration in the Internal Ignition test was significantly less than concentrations detected during the External Ignition Test. This was determined to be due to the lesser number of battery cells that became involved in combustion during the Internal Ignition Test. However, HF

concentrations in both the Internal and External Ignition Tests were identified to be more than the PEL of 3 ppm (which is averaged over an 8-hour work shift) [125].

7.1.9. Bordes et al., 2022

In this study, a series of tests was conducted on NMC pouch cells in various configurations to compare heat generation and gas and particle emissions during flaming thermal runaway versus non-flaming thermal runaway. The cells utilized in all tests were NMC pouch cells at 100% SOC with a nominal capacity of 70 Wh and a total mass of 485.3 g. The percent mass composition of a prototype cell was found to be 31% positive electrode materials and additives, 18% current collectors, 23% electrolyte, 4% separator, and 7% packing materials and connectors. All tests were conducted within a chamber with gas sampling extracted from the exhaust duct, with gas analysis performed through NDIR for CO and CO₂, a chemiluminescence-based on-line analyzer (CLD) for NO_x, FID for total hydrocarbons, and FTIR for additional gases such as organic carbonates (EC, DMC, EMC), aldehydes, and fluorinated species (HF and PO₂F₃). Air flow rates in the test chamber were approximately 1,000 m³/h for the cell level test and 2,000 m³/h for the array and module level tests. A PTFE filter was placed within the test chamber for particle sampling of aluminum, cobalt, copper, lithium, phosphorus, nickel, and manganese with analyses by ICP-OES. A cellulosic filter was placed within the test chamber for particle sampling of fluorinated species with analyses according to the NF X 43-304 French standard.

HRR and total effective heat of combustion were determined through CO and CO₂ generation calorimetry. The authors note that, in thermal runaway incidents, this method does not account for heat loss due to electrical or chemical processes, which might contribute up to 1/3 of the total thermal energy released in such an incident.

The first test was a cell-level test with thermal runaway initiated by an internal heater. Two insulated plates were placed on either side of the cell. During the test, the cell was observed to emit gases, without ignition, for the majority of the incident duration. A brief ignition of the vented gases occurred but did not result in a sustained flaming condition. Venting of gases during thermal runaway occurred for approximately 4 seconds. The maximum vent gas temperature recorded was 410°C. The total gas released was 38 L (0.5 L/Wh). The authors reported the quantity of gases measured for the NMC pouch cell test.

The second test was on a three-cell array, with the cells arranged in parallel and separated by aluminum plates. The cell array was partially encased with a polymer compression pad and acrylonitrile butadiene styrene (ABS) plastic. The total nominal capacity of the array was 210 Wh. Thermal runaway was initiated via an internal heater on the central cell. The initiating cell was observed to vent gas, which briefly ignited, and then gas emission became minimal. Propagation of thermal runaway to a second cell occurred 110 sec after the first cell entered thermal runaway. The third cell entered thermal runaway 180 sec after the second cell. Once the second cell became involved, flaming became more significant and sustained. The total gas released was 350 L (1.7 L/Wh). The authors reported the quantity of gases measured for the NMC pouch array test.

The third test was considered a module scale test and consisted of three, 3-cell arrays arranged in series. Each 3-cell array was separated by a polymer compression pad and an aluminum plate. The ends of the cells were partially encased with ABS plastic. The total nominal capacity of the array was 627 Wh. Thermal runaway was initiated via an internal heater on the central cell. The initiating cell was observed to release significant gas, then calm down for 60 sec. The module then

exhibited violent behavior, with strong flames, as the two adjacent cells simultaneously entered thermal runaway. Flaming conditions, due to the plastic components of the module, was observed up to 25 min after the first cell entered thermal runaway. During the test, thermal runaway only propagated through the initiating cell array. The other two cell arrays, on either side of the initiating array, moderately increased in temperature, but did not enter thermal runaway. The authors attributed this to the polymer/aluminum barriers between the arrays. The total gas released was 466 L (0.8 L/Wh). The authors note that the quantity of gases is only from three of the nine cells in the module. Therefore, they provide a corrected normalized gas emission on 2.2 L/Wh. The authors reported the quantity of gases measured for the NMC module level test.

Bordes et al. (2022) noted that CO₂, HF, and NO_x increased with the occurrence of flaming conditions, while methane, ethylene, CO, POF₃, carbonates, formaldehyde, and H₂ decreased. The authors contributed the increase in HF production during flaming conditions to the increase in temperature, which encourages thermal decomposition of fluorinated compounds, and/or the production of water which promotes HF formation from POF₃. This was also used to explain the decreased presence of POF₃ during flaming conditions with an increase during lower temperature and lower HRR conditions. The decrease of hydrocarbons during the flaming stages was contributed to these gases becoming involved in the combustion. Production of NO_x was noted only in the array and module level tests, and this was determined to be due to the presence of the ABS plastic encasing, which was not included in the cell level test.

The total heat released for the cell, array, and module tests were approximately 0.5, 8.0, and 10.5 MJ, respectively. For the array and module level tests, the heat released from the cells was estimated to be the same, however, the additional 2.5 MJ in the module test was produced during the slow combustion of plastic components of the module after completion of thermal runaway.

Bordes et al. (2022) determined an effective heat of combustion of 6 to 12 kJ/Wh for non-flaming conditions and 50 kJ/Wh for flaming conditions. This was explained by flaming conditions supporting a more effective thermochemical process, the involvement of additional combustible items (i.e. plastics, separators) during flaming conditions, and the increase of available oxygen. The peak HRR during the array test was found to be 130 kW, when the third cell entered thermal runaway. The peak HRR during the module test was found to be 250 kW, when the second and third cells entered thermal runaway simultaneously. In both tests, the HRR during thermal runaway of the initiating cells, with no flames present, was found to be 20 to 25 kW.

Regarding inorganic particle emissions from the three tests, nickel manganese, and cobalt were found to be the most prevalent, which represent the cell's electrode chemistry. The authors reported the mass composition of the inorganic particles collected during the tests. The mass composition is understood to exclude organic particles, such as carbon [63].

7.1.10. Bordes et al., 2024

To determine the environmental impact of firefighting during Li-ion thermal runaway incidents, Bordes et al. (2024) analyzed the firewater runoff from prismatic and 18650 battery modules. The prismatic module (Module A) contained 16 NMC cells rated for 500 Wh. The 18650 module (Module B) contained two cell blocks with 45 cylindrical, NMC cells (90 cells total) rated for 900 Wh. Modules were forced into thermal runaway using a gas burner or thermal pads and positioned under a sprinkler. For each test, 2 L of the firewater runoff was sampled and exposed to direct flame to remove potential organic solvents.

ICP-OES was used to analyze aluminum, iron, lithium, sodium, nickel, and phosphorus. ICP-MS was used for cobalt, copper, and manganese. Chlorine and fluorine were detected using ion chromatography. Liquid chromatography was used to quantify PAH. Carbonates were analyzed using gas chromatography and a flame ionization detector. The centrifugal disc method was used to determine particle size distribution.

Tests 1 and 2 involved Module A and were both extinguished using 7 L of water. In Test 1, there was venting and moderate fire, but the module casing did not open. Due to the moderate damage, the authors decided to push the same module into thermal runaway in Test 2. The module produced jet fire and exploded, damaging all cells and the casing. The water collector was not emptied between tests and water was sampled after the conclusion of each test. The total water applied was 14 L. Test 3 involved Module B and was extinguished using 9 L of water. Module B produced jet fire and exploded, burning all cells. The authors reported the concentrations of the contaminants found in the firewater runoff.

The authors noted that the transition metals found in the cathode (nickel, manganese, and cobalt) were more prevalent with increased severity of the thermal runaway. Nickel was found in larger quantities than manganese and cobalt, which was representative of the NMC cell composition. Fluorine, chlorine, and lithium from the cell electrolyte and electrode were found. The authors also noted that while aluminum, copper and iron were found, they were present in sheets or bulk form, which indicates that it was less likely to be found in particle emissions. Bordes et al. also noted that the cooling effect of the water could lead to a higher concentration of organic carbonates. Furthermore, carbonates were only found in Tests 1 and 2, possibly due to the higher temperatures produced in Test 3 which could have led to total decomposition of the carbonates.

Only Test 1 produced particles around 70 nm. Tests 2 and 3 primarily had particles ranging from 0.9 to 2 μm . Bordes et al. concluded that this distribution was possibly due to the nanoparticles being carried away by the plume before the extinguishing water could reach them. The nanoparticles in Test 1 were primarily composed of fine particles a little smaller than 100 nm. The largest particles were around 1 μm and composed of iron and aluminum.

The authors extrapolated the concentrations found in their tests to a real-life incident involving a 1,500 kWh BESS fire. The concentrations were normalized by capacity. In Test 1, the water poured per capacity was 0.014 L/Wh. Tests 2 and 3 had 0.024 L/Wh and 0.01 L/Wh poured, respectively. The concentrations were compared to the PNEC values for wastewater established by the ECHA⁹. Concentrations of cobalt and EMC were particularly high (2500 and 260 times greater, respectively). The authors also noted that the concentration regulations found from other sources for some elements, such as nickel, were lower than the values provided by ECHA. They also noted that potential interactions between the chemicals had not been thoroughly explored. Researchers concluded that firewater runoff contained metals, carbonaceous materials, and in some cases, electrolyte solvents. Almost all contaminant concentrations exceeded the PNEC values; as such, researchers concluded that firewater runoff from a large-scale incident could be hazardous to the environment [109].

⁹ The PNEC is the level below which an adverse effect to an ecosystem is unlikely regardless of exposure duration. ECHA is only one source for PNEC values.

7.1.11. Chen et al., 2017

Chen et al. (2017) performed testing on Li-ion batteries to assess the toxicity of the gases released during flaming thermal runaway. The test was conducted in accordance with the Chinese test standards GB/T 8323.2 and TB/T 3237-2010. The batteries were exposed to a 25 kW/m² radiant heater and ignited with a pilot flame inside a chamber. Gases released were measured via infrared analyzing instrumentation (CO and CO₂) and colorimetric gas detector tubes (SO₂, HCl, HBr, HF, HCN, NO_x). The specifications of the batteries were not identified. The results of the analysis are reported by the authors. Chen et al. (2017) determined that the gases were within a safe concentration range and “qualified.” However, it is unknown what criteria were used to reach this conclusion. The gas concentrations were assessed for toxicity using the Chinese National Standard GB/T 20285-2006. Mice were exposed to the smoke and toxic gases produced. If the mice died within 30 minutes of exposure or had continued weight loss, the gas was considered dangerous. If the mice recovered to their initial weight within three days and were still alive, the gases would be considered safe enough to have the highest allowable smoke concentration limit. The gases were ranked ZA2 and were “qualified.” However, the authors do not explain what these classifications indicate. Absent battery specifications, it was not possible to correlate the gases produced with cell chemistry [126].

7.1.12. Gully et al., 2019

To assess Li-ion battery explosion risk and effectiveness of fire suppression methods, DNV GL conducted a series of tests on NMC and LFP cells to quantify gas production during thermal runaway events. Cell level tests were conducted with NMC pouch cells with a capacity of 63 Ah, LFP cylindrical 18650 cells with a capacity of 1.5 Ah, and LFP cylindrical 26650 cells with a capacity of 2.5 Ah, at varying SOC.

The tests were conducted inside a 0.44 m³ chamber equipped with an exhaust fan set to flow air at a rate of 11 L/s. Gas samples were obtained from the interior of the chamber and FTIR was used for analysis of gases including CO, CO₂, NO, NO₂, HCl, HF, HCN, methane, ethane, ethylene, benzene, toluene, ethanol, and methanol.

CFD modeling was used to estimate the total amount of gas produced in the chamber, based on the FTIR concentration measurements. The CFD model did not account for leakage from the chamber. In addition, due to limitations of the measuring equipment, the results do not include hydrogen. However, using an assumed hydrogen concentration value of 30 %vol, based on a literature review, the authors adjusted the estimated total amount of gas produced; the authors did not adjust the toxic gas concentration estimates. The authors reported the adjusted total amount of gas produced for each test as well as the unadjusted percent volume concentration of toxic and asphyxiant gases. It was noted that generally, tests in which there was no visible combustion, a greater quantity of gas was produced, due to an increase in CO and CO₂.

It was observed that the NMC cells produced their own oxygen during combustion of the electrodes, which encouraged flaming conditions, and likely contributed to increased yields of CO and CO₂. NMC cell tests also experienced higher temperatures and faster temperature increases. The duration of the intense vent gas release period at thermal runaway was found to be between 40 to 50 seconds for the NMC cells when flaming conditions was present, but this duration increased to 150 and 1050 seconds in cases where there were no flaming conditions.

For NMC cells, the thermal runaway onset temperature was found to be between 173 and 250°C for overheat failure scenarios and the maximum cell temperature was 481°C. For the overcharge and short circuit failure scenarios for NMC cells, the thermal runaway onset temperature was found to be 80 and 30°C, respectively, and the maximum cell temperature was 602°C. For the 1.5 Ah LFP cells, the thermal runaway onset temperature was found to be between 210 and 225°C for overheat failure scenarios and the maximum cell temperature was 384°C. The maximum cell temperature for the 2.5 Ah LFP cells was 243°C; the thermal runaway onset temperature could not be identified for these tests. For NMC cells, the temperature increase rate across all tests was between 13.6°C/s and 229°C/s, while for the LFP cells, the temperature increase rate across all tests was between 0.14°C/s and 5.06°C/s.

DNV GL also conducted a series of tests on NMC and LFP modules. Gas volume and gas concentrations were not reported for these tests. However, the authors observed that non-flaming scenarios produced more gas than flaming scenarios, consistent with what was observed in the cell level tests [57].

7.1.13. Ditch & Zeng, 2020

In a study conducted by Factory Mutual (FM), small, intermediate, and large-scale fire tests of Li-ion battery modules and module racks were performed. The tests were performed with two types of battery cell chemistries, LFP and LNO/LMO. The LFP cells had a 0.07 kWh capacity. The LNO/LMO cells had a 0.12 kWh capacity. The modules and racks for each battery type were set up in similar configurations. Modules were rectangular and made up of prismatic cells, arranged in a single row with thin metal cooling plates separating each cell. All modules were tested at a SOC of at least 95%. The LFP module contained 78 cells with a total capacity of 5.2 kWh and a total mass of 49 kg with a combustible load of 7.5 kg. The LNO/LMO module contained 64 cells with a total capacity of 7.8 kWh and a total mass of 75 kg with a combustible load of 13.6 kg. Racks were constructed with 8 levels of two modules side by side, for a total of 16 modules per rack, with the sides and backs of the rack enclosed with sheet steel. The LFP rack contained 1,248 cells with a total capacity of 83.6 kWh. The LNO/LMO rack contained 1,024 cells with a total capacity of 125 kWh. A thin removable separator, plastic for LFP tests and aluminum for LNO/LMO tests, was installed between the two columns of modules within the rack. The front of the rack was left open. The battery management system for the rack was in place at the top of the rack but was not active during the tests; as such, protective mechanisms that would normally detect and shut down the unit during thermal runaway were not operational.

The total combustible load of the modules and racks were estimated based on total weights and estimated mass percentages of the combustible components, classified into either electrolyte or unexpanded plastics. Electrolyte mass was estimated to be 7% of the individual battery mass, based on the author's experience in studies of batteries with similar capacity, and approximately 15 to 20% of the total module mass was classified as combustible. The material and mass of the separators within the battery cells were unknown and therefore not included in the calculations for combustible loads. The remainder of the module components were mostly metal and considered negligible. For the electrolyte heat of combustion, a value of 28 MJ/kg, based on DEC, was used and for the plastic components a value of 38 MJ/kg was used. A $\pm 10\%$ uncertainty was added for the calculated energies. The calculated total combustible load was approximately 279 MJ for the LFP module and 4,464 MJ for the rack. The calculated total combustible load was approximately 509 MJ for the LNO/LMO module and 8,142 MJ for the rack.

Tests were performed under a hood to measure the HRR of the various fire tests through three different techniques. The convective HRR was calculated from the measured gas temperature and mass flow through the FPC. An uncertainty of $\pm 10\%$ was applied to these results. The chemical HRR was calculated from the measurement of CO and CO₂ within the hood duct. An uncertainty of $\pm 20\%$ was applied to these results to account for typical sources of uncertainty for ordinary combustibles as well as carbonate species produced during thermal runaway. Ditch and Zeng (2020) identified that previous studies have suggested that HRR rate calculations based on oxygen consumption can be corrected to account for the thermal runaway gases produced by Li-ion batteries; however, they determined that these corrections could not be accurately applied in their tests due to variability based on battery chemistry, quantities of batteries, quantity of other combustibles, and stages of fire development. Chemical HRR based on oxygen consumption calorimetry was also calculated for the tests but was found to be unreliable due to drifting of the O₂ analyzer; as such, these results were not reported.

In the small-scale tests, a single battery module was forced into thermal runaway via heating elements attached to the underside of the module. The heating source remained active until sustained burning was achieved within the module. In the LFP tests, it was observed that while significant vent gases were released during heating, ignition of these gases did not always occur, and had to be initiated via an external pilot flame in some cases. When self-ignition did occur, the time to ignition varied from 45 seconds to 7 minutes after venting. Meanwhile, in the LNO/LMO cell tests, sparks and flames were observed that consistently ignited the cell vent gases.

The LNO/LMO module was observed to produce a much higher peak chemical HRR (1,023 kW) and chemical THR (315 MJ) compared to the LFP module (413 kW and 143 MJ, respectively). The corresponding convective HRR and THR values were 450 kW and 204 MJ for the LNO/LMO module and 214 kW and 101 MJ for the LFP module. These values were approximately 50-60% of the estimated combustible load energies discussed previously.

In the intermediate-scale tests, three levels of two battery modules side by side were installed within a metal cabinet, for a total of 6 modules. Based upon the description, it is assumed that there was no metal dividers or separations between the stacks. The bottom left module was forced into thermal runaway via heating elements attached to the underside of the module. A pilot flame, intended to ensure ignition of cell vent gases, was placed at the bottom of the rack 76 mm from the face of the initiating module. A pilot flame was not used for the single module testing.

For the LFP modules, it was observed that from the initiating module, the fire spread vertically up the left stack. After the top left module ignited, fire spread horizontally to the top right module (approximately 40 minutes after first sustained flames observed at initiating module), and then spread downwards to the two remaining modules in the right stack. The fire reached the peak HRR approximately 84 minutes after the first sustained flames were observed at the initiating module. In total, the fire burned for over 150 minutes before it was manually extinguished prior to all fuel being fully consumed. For the LNO/LMO modules, from the initiating module the fire spread horizontally to the bottom right module. Then, the fire spread vertically and simultaneously up both modules. The LNO/LMO peak HRR was reached at approximately 32 minutes after sustained flames were observed at the initiating module. All LNO/LMO modules were observed to be burned out at 74 minutes after sustained flames were observed at the initiating module; however, an orange glow continued until the test was terminated 72 minutes later.

The LNO/LMO modules were observed to produce a much higher peak chemical HRR (1,890 kW) and chemical THR (2,034 MJ) compared to the LFP modules (500 kW and 1,152 MJ, respectively). The corresponding convective HRR and THR values were 1,020 kW and 1,435 MJ for the LNO/LMO module and 312 kW and 758 MJ for the LFP module. These values were approximately 66% of the estimated combustible load energies discussed previously. It was estimated that an additional 5% of total heat released could be added to the LFP module test given that the fire was extinguished before full mass consumption.

The large-scale tests were run in the same manner as the intermediate-scale tests, except that a full BESS rack was used. The rack was provided by an unidentified manufacturer and populated with eight levels of two modules side by side for a total of 16 modules. Imitation rack extensions were installed on either side of the rack but were not populated with additional battery modules. For both the LFP and LNO/LMO racks, from the bottom left initiating module, the fire was observed to spread vertically up the center of the rack igniting modules on both sides. For the LFP rack, the peak HRR was reached at approximately 34 minutes after sustained flames were observed at the initiating module. The fire burned for approximately 98 minutes before self-extinguishing. For the LNO/LMO rack, the peak HRR was reached at approximately 29 minutes after the sustained flames were observed at the initiating module. The fire burned for over 160 minutes before it was manually extinguished, prior to all fuel being fully consumed.

The LNO/LMO rack produced a much higher peak chemical HRR (10,660 kW) and chemical THR (6,390 MJ) compared to the LFP rack (2,540 kW and 3,810 MJ, respectively). The corresponding convective HRR and THR values were 6,840 kW and 4,660 MJ for the LNO/LMO module and 1,680 kW and 2,770 MJ for the LFP module. These values were approximately 78 to 85% of the estimated combustible load energies discussed previously.

The results from all three levels of tests were analyzed to identify relationships between electrical capacity of the battery installation, combustible load, total energy released, and peak HRRs. It was found that total energy released had a linear relationship with both electrical capacity and combustible load, and trends were consistent across the LFP and LNO/LMO batteries. However, it was found that the peak HRR had a non-linear relationship with both electrical capacity and combustible load, and trends were different across the LFP and LNO/LMO batteries. This non-linear trend was partially attributed to the occurrence of more extensive heating in the rack and multi-module systems which lead to more rapid involvement of subsequent modules. Ditch and Zeng (2020) noted that the trends identified in their testing should not be universally applied to other batteries, modules, or systems. The reason was because different battery modules, even those that are LFP or LNO/LMO, may have different ratios of electrical capacity to combustible load and/or different energy capacities per unit of volume [13].

7.1.14. Essl et al., 2020a

In this study, a series of tests on NMC/LMO cells was conducted to investigate hazards related to thermal behavior, vent gas production, and vent gas composition. The cells utilized were 41 Ah/156 Wh, NMC/LMO pouch cells at 100, 30, and 0% SOC. The cell mass was 865 g. The experiments were conducted inside a pressure chamber, purged with nitrogen. Thermal runaway was initiated by heater stripes attached to the metal sample holder plates on either side of the cell. Thermocouples were placed in four locations within the chamber to measure gas temperatures. Vent gas production was determined through pressure sensors in the chamber and the ideal gas

law. Total gas production was determined for the total duration, between the initial vent and the initiation of thermal runaway, during thermal runaway, as well as the venting rate when 50% of the vent gas is released. The composition of the vent gases was determined via FTIR and gas chromatography. Gases analyzed were H₂, CO, CO₂, methane, ethane, ethylene, acetylene, DEC, DMC, EC, EMC, H₂O, hexane, HF, butane, and propane.

The thermal runaway onset temperature was determined to be 170°C for the 100% SOC cell. The experiments involving the 30% and 0% SOC cells did not achieve thermal runaway. The authors observed that the vent gas composition reported in the 30% and 0% SOC tests was similar to that found prior to thermal runaway in the 100% SOC test. HF was not detected in any of the tests [64].

7.1.15. Essl et al., 2020b

Essl et al. (2020b) performed a series of tests on NMC cells to understand how different thermal runaway triggers influenced thermal behavior, vent gas production, and vent gas composition. Two types of cells were utilized, a 60 Ah/216 Wh, NMC prismatic cell at 100% SOC and a 60 Ah, NMC pouch cell at 100% SOC. The prismatic cells had a EC:DMC:EMC electrolyte and the pouch cells had a EC:EMC electrolyte. The experiments were conducted inside a pressure chamber, purged with nitrogen. Thermal runaway was initiated by overtemperature, overcharge, and nail penetration. Thermocouples were placed in the pouch cell's foil welded sides and at the prismatic cell burst plates to measure the vent gas temperatures. Vent gas production was determined through the use of pressure sensors in the chamber and the ideal gas law. Quantities of gas were determined for the total duration, between the initial vent and the initiation of thermal runaway, during thermal runaway, as well as the venting rate when 50% of the vent gas is released. The composition of the vent gases, only after thermal runaway, was determined via FTIR and gas chromatography. Gases analyzed were H₂, CO, CO₂, methane, ethane, ethylene, acetylene, DEC, DMC, EC, EMC, H₂O, hexane, HF, butane, and propane.

The average maximum vent gas temperatures for the pouch cells were 584°C, 1044°C, and 482°C, for the overtemperature, overcharge, and nail penetration failure scenarios, respectively. The average maximum vent gas temperatures for the prismatic cells were 1169°C, 1021°C, and 850°C, for the overtemperature, overcharge, and nail penetration failure scenarios, respectively. The authors noted that the increase in the vent gas temperatures seen for the prismatic cells was due to a more concentrated point release from the cell, as opposed to the pouch cells where the gas can release simultaneously from all sides. The authors also noted that the vent gas temperature might be influenced by the ejection of hot particles.

The authors noted that while HF was not detected in any of these tests, they assume that it was produced in small amounts but due to the high reactivity of the compound, it did not transport into the FTIR spectrometer. It was also noted that the same experimental setup was used for older 18 Ah NMC/LTO cells and a concentration of 66 ppm of HF was detected after thermal runaway. The authors identified that the detection of EC was highly unlikely with the experimental setup. The overcharge experiments were observed to generate significantly more gas, have a higher mass loss, and have a higher concentration of H₂ and CO. The authors suggested this is due to the additional energy that is imparted into the cells by the overcharge [65].

7.1.16. Forestier et al., 2020

In an evaluation of the influence of Li-ion battery cell confinement, electrolyte composition, and separator composition on thermal and toxicological hazards, Forestier et al. (2020) performed a series of tests on 0.6 Ah NMC pouch cells. The total mass of the cell was approximately 13.5 g and consisted of approximately 31% negative electrode, 20% current collectors, 18% electrolyte, 4% separator, and 9% packaging materials and connectors.

Tests of single cells were conducted within a chamber filled with ambient air. Thermal runaway was initiated via heating wire with a continuous ramp. Gas sampling and analysis was performed via a heated sampling line from the top of the chamber connected to a FTIR spectrometer.

Thermal runaway onset temperatures were determined to be 180 to 200°C when the cells were not confined with pressure, and 245°C when pressure was applied. The authors explained that the increase in onset temperature in the confined case is due to the restriction of cell swelling which prevents electrolyte from coming into contact with the electrodes. The authors reported the results of the gas analysis for certain groups of tests. The publication did not report specific values for each test conducted. The authors noted that the confined cell tests (pressure applied to sides of cell) produced less gas overall, including both hydrocarbons and toxics. This was also contributed to the cell not being allowed to swell, thus preventing additional electrolyte from coming into contact with the electrodes [127].

7.1.17. Franqueville et al., 2023

Franqueville et al. (2023) assessed the minimum safety distances related to firefighting and evacuation for Li-ion thermal runaway incidents. A meta-analysis of the literature was conducted to establish the main toxic gas species emitted by Li-ion batteries. CFD modeling was performed using FDS to characterize toxic gas profiles associated with various ambient conditions, e.g., temperature, wind, etc., and battery characteristics. Estimated minimum safety distances were determined through comparison of predicted toxic gas concentrations and IDLH values.

The production of toxic gases was modeled as a boundary condition with mass flow rate for the lumped toxic gas species. The mass flow rate was calculated by multiplying the sum of estimated yields for each species by an estimated total mass production rate. For lumped species, the fraction of each toxic gas was specified using mass fractions that were proportional to the yields. The yield of each toxic species was obtained by dividing its reported mass production per unit of battery energy by the estimated total mass produced per unit of battery energy. The mean mass of gas produced per unit of battery energy was 0.47 g/Wh. An estimated heat of combustion was derived using experiments where the total heat released, and mass loss was reported. The heat of combustion was found to be 17 MJ/kg. The mean mass loss per unit battery energy was 2.3 g/Wh. To calculate the distribution of HF yields, the HF data reported in terms of mass per unit of battery energy were divided by the approximate total mass released per unit of battery energy.

A model representing a home garage, or the container of a BESS unit, was run for both flaming and non-flaming thermal runaway. The room was 6 m by 5 m by 2.5 m with a 1 m by 2 m open door. A 4 m by 1 m by 1 m object representing a battery was placed inside the room. There were two vents on the battery, one for toxic gases and the other for flammable gases. The domain size

was 36 m by 104 m by 8 m and the sides and top were set to open. The grid inside the room was 25 cm, and was increased to 50 cm, 1 m, and 2 m outside the room.

Refining the mesh did not significantly change the plume characteristics. The concentration field of each toxic gas was extracted at 2 m to represent head height. The maximum battery system size was set to energy of 3.1 MWh at 100% SOC. The mean HF value used was 0.008 kg/kg for non-flaming; HF was only gas coming out of the toxic vent. Mean volume percentages of all other species including CO, CO₂, and H₂, were assigned to the flammable gases vent. The gas release temperature was 300°C.

For flaming, the gas released normalized by capacity in Wh was determined by applying a multiplier five to the non-flaming case. The FDS “simple” combustion model was used. The gases released from the toxic vent were HF, CO, HCl, NO, and SO₂. The release of these toxic gases was defined by a lumped toxic gas species and composition was specified using mass fractions. The MLR of the lumped toxic gas species was specified by multiplying the total mass flow rate by the sum of the yields of all toxic gases. The soot yield was set at 0.05 kg/kg. The MLR profiles are triangular and ranged from 1 kg/s (non-flaming) to 4 kg/s (flaming) at peak. The steady state equivalent MLR was approximately 1 kg/s for the flaming and non-flaming cases.

The flaming simulation used a summed toxic gas yield rather than an individual yield. Scenario-based simulations included 50 and 100% SOC, wind speeds of 3, 8, 24, and 32 km/h, and six battery energies ranging from 5 kWh to 3 MWh. Zero mph wind cases were not considered because it showed that the plume went straight up, so safety distances were very small, e.g., the smaller the safety distance, the closer the firefighter can be to the source without a negative health impact. Failure duration was one hour.

A battery electric vehicle (BEV) was modeled using yields from the vehicle that produced the most toxic concentrations. The computational domain and room sizes remained the same as the BESS unit model.

For the non-flaming case, the worst-case timestep regarding toxicity was at the peak mass flow rate. However, the worst-case timestep in the flaming case did not align with the peak mass flow rate. The authors determined this was due to a balance between two factors; as the HRR increased, plume buoyancy increased and reduced the safety distance while at the same time, the mass flow rate of the toxic gases increased, causing an increase in safety distance. The authors identified that when the mass flow rate is less than 1 kg/s, the effect of toxic gas mass flow dominates, and the safety distance increases with the mass flow rate. The study found that plumes in the 100% SOC scenarios had a greater buoyancy than in the 50% scenario, which would decrease safety distances. However, the increased toxic gas production outweighed this effect, resulting in an overall increase in safety distances for 100% SOC scenarios versus 50% SOC scenarios.

For all flaming simulations, HF was the gas setting the safety distance. HF was the gas that required the largest distance to drop below IDLH. The largest safety distances across all SOC and battery sizes for the 2, 5, 15, and 20 mph wind speeds were 5, 13, 45, and 54 m, respectively. The authors contributed the correlation of increasing safety distance with increasing wind speeds to the plume being able to rise upwards at the low wind speeds.

For the non-flaming scenarios, most safety distances were also set by HF. The largest safety distances across all SOC and battery sizes increased from 13 m to 51 m at 2 mph and 5 mph, respectively but then decreased to 34 m and 22 m at 15 and 20 mph, respectively. The authors

contributed the decrease in safety distance at high wind speeds to increased dilution of the plume. In all cases, the non-flaming scenarios had higher or approximately equal mean safety distances compared to the flaming scenarios [47].

7.1.18. Golubkov et al., 2014

Golubkov et al. (2014) conducted thermal runaway experiments on three types of Li-ion cell chemistries to evaluate the influence of cell chemistry on the thermal and explosive hazards. The cells utilized were LCO/NMC cells with a 2.6 Ah/9.9 Wh capacity and a mass of 44.3 g, NMC cells with a 1.5 Ah/5.7 Wh capacity and mass of 43.0 g, and LFP cells with a 1.1 Ah/3.5 Wh capacity and a mass of 38.8 g. All cells were cylindrical 18650 type cells at 100% SOC.

The experiments were conducted inside a sealed reactor, purged with argon. Thermal runaway of the cells was initiated by a heating sleeve with a consistent temperature ramp. Gas temperatures and pressure inside the reactor were measured and inputted into the ideal gas law to determine the quantities of gas produced. Gas samples from the chamber were started after thermal runaway or, if no thermal runaway occurred, after the cell temperature exceeded 250°C. Gas samples were analyzed for H₂, O₂, N₂, and hydrocarbons using gas chromatography. The authors reported the thermal runaway onset temperature, vent duration, quantity of vent gas produced, and the CO₂ and CO mole percentages of the vent gas for each for each cell chemistry [58].

7.1.19. Golubkov et al., 2015

In this study, Golubkov et al. (2015) performed testing of LFP and NCA Li-ion cells to assess the impact of SOC and overcharge. The cells utilized in the testing were all 18650 cylindrical cells. The LFP cells had a mass of 38.87 g and a nominal capacity of 1.1 Ah. The NCA cells had a mass of 45.4 g and a nominal capacity of 3.35 Ah. The LFP cells were charged to 3.5V and the NCA were charged to 4.2V.

The experiments were conducted inside a sealed reactor, purged with inert gas (nitrogen or argon). Thermal runaway of the cells was initiated by a heating sleeve with a consistent temperature ramp. Gas temperatures and pressure inside the reactor were measured and inputted into the ideal gas law to determine the quantities of gas produced. Gas samples from the chamber were started after thermal runaway or, if no thermal runaway occurred, after the cell temperature exceeded 250°C. Gas samples were analyzed for H₂, O₂, N₂, and hydrocarbons using gas chromatography.

NCA and LFP Cells with a 0% SOC did not enter thermal runaway and displayed vent gas releases with a uniform rate; there were no sudden or violent reactions or gas releases. NCA cells with a SOC of 25% or greater did enter thermal runaway. LFP cells with a SOC of 25% did not achieve distinctive thermal runaway and behaved similar to the 0% SOC. LFP cells with a SOC of 50% or greater did enter thermal runaway. Thermal runaway onset temperatures for LFP and NCA cells with a SOC of 100% or less were between 136 and 160°C. Thermal runaway onset temperatures for NCA cells with a SOC of greater than 100% were between 65 and 80°C, while for overcharged LFP cells they were still approximately 140°C. The authors reported the mass loss, quantity of vent gas produced, and the CO₂ and CO mole percentages of the vent gas for all tests.

The authors noted that for NCA cells, the quantity of gas increased with increasing SOC; however, for LFP cells, there was not a clear correlation. For NCA cells, as the SOC increased, the concentration of CO tended to increase while the concentration of CO₂ decreased. For LFP cells, as the SOC increased, the concentration of CO₂ decreased. CO concentrations were observed to be lower for LFP cells (maximum 9.1 %) versus NCA cells (maximum 49.2%) [59].

7.1.20. Held et al., 2022

Held et al. (2022) performed experimental testing of Li-ion thermal runaway to analyze the potential for soot to settle and contaminate a surrounding enclosed space. Gas analyses were not included in the study. The tests utilized a battery module made up of 12 prismatic, Samsung SDI, 90 Ah, NMC cells at 100% SOC. The anode material of the cell was graphite, the electrolyte was organic carbonates with LiPF₆ salts. The module was rated for 4.15 kWh at 44V (3.68 V per cell) and had a mass of 29.6 kg. All 12 cells of the module were forced into thermal runaway simultaneously in each of three test scenarios.

In test scenario 1, the module was forced into thermal runaway within a 250 m³ enclosure without ventilation and without extinguishment. Stainless steel collector plates were placed at heights of 1 and 3 meters and tilted 45 degrees towards the experiment. A firefighter's protective suit (93% Nomex) was also placed in the enclosure. The same enclosure was used in test scenario 2, but to assess the impact of water application, a sprinkler (with a flow rate of approximately 20 L/min) was installed in the enclosure. The burning battery module was shielded from the sprinkler to assess only the deposits from soot and smoke in the water. The water flowed from the sprinkler, a total of 280 liters during the test, was all collected in a container. In addition, at the conclusion of the test and for separate analysis, the burned battery was placed in a container which was then filled with 50 liters of water. In test scenario 3, the module was forced into thermal runaway within a 160 m open tunnel with a defined airflow of 1.5 m/s. Stainless steel collector plates were placed at a height of 3.5 meters and tilted 5 degrees against the airflow at distances of 50, 100, and 150 meters from the battery.

Soot samples were analyzed via SEM-EDX and ED-XRF for elemental composition. The results of the tests showed that the Li-ion battery module fire produced soot composed mainly of heavy metal-oxides of nickel, manganese, and cobalt (each 18 to 20 %mass). Also present were lithium (3 to 4 %mass), fluorides (2.4 %mass), and chlorides (.2 %mass). Concentrations were identified to exceed usual background levels by a factor of 2000-4000 for cobalt and nickel, 500 to 700 for manganese, 400 to 700 for lithium, and 50 for fluorides. PAH quantities were found to be approximately 250 to 300 µg/m² on stainless steel collector plates and 120 µg/m² on the firefighter's protective gear; these levels were noted to be approximately 50 and 20 times the measured background limits, respectively, and up to 3 times the restoration goal for industrial environments. Polychlorinated biphenyl (PCB) and polychlorinated dibenzo-p-dioxin and furan (PCDD/F) quantities were not found to be elevated above the normal background range. The water analysis from test scenario 2 showed that the same substances were dissolved in the water, particularly the heavy metals. The drinking water limits, and industrial effluent limits provided in the study are those decreed in Switzerland (or Germany), not the United States.

In the water collected from the sprinkler, levels of sulphates, chlorides, and nitrates were below the drinking water limits in Switzerland. The lithium level was found to exceed the drinking water limit in Germany by a factor of 80. Switzerland does not have a limit for lithium, so the Germany

limit was used. The levels of nickel, cobalt, and manganese were found to exceed Switzerland's drinking water limits by factors of 700 to 1,800. For the water into which the battery was submerged (Storage Water), extremely high concentrations of metals and fluoride were found. Organic substances produced by the fire such as PAH, PCB, and PCDD/F were all detected at very low concentrations or below detection limits. The levels of nickel, cobalt, and manganese were found to exceed Switzerland's drinking water limits by factors of 1,000 to 2,800.

Results from test scenario 3 showed that, with the application of ventilation, the soot settled at a much lesser density throughout the test tunnel ($<0.5 \text{ g/m}^2$) compared to the non-ventilated enclosure ($17 \text{ to } 20 \text{ g/m}^2$). The concentration of cobalt, nickel, and manganese were also less at 7 to 9% by mass compared to 18 to 20% by mass found in test scenario 1. However, concentrations were still identified to exceed usual background levels by a factor of 50 to 200 for cobalt and nickel, 5 to 20 for manganese, and 10 to 30 for lithium. Fluoride levels measured in test scenario 3 were negligible [110].

7.1.21. Hill, 2020

On April 19, 2019, a thermal runaway event occurred in a McMicken BESS in Surprise, Arizona. The report by Hill (2020) discusses the findings of the incident investigation and subsequent analysis and provides background on typical Li-ion battery characteristics. The unit involved in the incident was a 2 MW/MWh battery composed of 10,584 NMC pouch battery cells manufactured by LG Chem. The pouch cells were Model JP3 and were 64 Ah/0.24 kWh cells with an operational voltage of 3.0 to 4.2V. The cells were arranged into 6.7 kWh modules with 28 cells per module. The modules were arranged into racks with 14 modules per rack. A total of 27 racks made up the BESS unit. The BESS was equipped with a clean agent fire suppression system. The incident was initiated when a single cell went into thermal runaway. The thermal runaway of the cell caused adjacent cells to go into thermal runaway, and eventually, spread to adjacent modules within the rack. Thermal runaway event, however, did not propagate to adjacent racks in the enclosure. Three hours into the event, firefighters opened a door to the unit and an explosion ensued; the explosion resulted from a buildup of combustible gases inside the unit during the thermal runaway and the introduction of oxygen into the enclosure through the open door.

An analysis of the incident was conducted to assess on-site and off-site environmental and health impacts. This analysis included collecting soil samples, surface samples, and performing air dispersion modeling to identify exposures to contaminants of concern. Soil samples were collected from the ground surface around the incident BESS, and wipe samples were collected from the interior of the BESS. These samples were analyzed for a variety of organic and inorganic compounds suspected to be present based on the chemical safety data sheets and information provided by the vendor. It was found that generally, within all samples, the concentrations of contaminants of concern were undetectable or like control samples. There were no samples that had concentrations greater than thresholds set by applicable state and federal standards for site remediation or response actions (Hill, 2020). Air dispersion modeling was conducted to assess the transport PM and contaminants of concern. The analysis "relied upon conservative emission rates", however, further details, including these emission rates were not provided in the report (Hill, 2020). The air dispersion modeling analysis concluded that PM dispersion was minimal and limited to the immediate area around the BESS and that concentrations of contaminants off-site were at levels below state and federal standards. The air dispersion modeling program employed was not stated [7].

7.1.22. Huang et al., 2016

The authors initiated thermal runaway in modules composed of NMC/LTO cells with a 50 Ah capacity at 100% SOC to characterize the thermal behavior of battery modules undergoing thermal runaway. Cells were equipped with tabs and relief valves set to vent at 0.5 MPa. Two different formations were tested- a rhombus and a parallel line. Both module types laid horizontally on a platform 85 mm above a 5-kW heater. A hood collected the combustion products. The authors measured HRR through oxygen consumption calorimetry, temperature at the cell surface and tabs, ambient temperature, and mass loss percentage to determine if the arrangement of the cells affected thermal runaway in the module.

For the rhombus module, a jet flame emerged from Cell 2 between 0 to 1601 seconds. At 2210 seconds, thermal runaway was triggered at the same cell, which caused a stronger jet flame and ignited Cell 4. However, the ignition of Cell 4 had no significant impact on the HRR. Cell 4 extinguished at the same time Cell 3 ignited and entered thermal runaway (2655 seconds). Jets of white and black smoke appeared from Cell 3. Then, the module entered a stable combustion phase lasting 120 seconds. Afterwards, there was no visible flaming/smoke ejection (2760 to 4011 seconds), but decomposition in all cells continued to produce combustible gases. At 4011 seconds, Cell 4 exploded, destroying the experimental set up. Two minutes later, Cell 1 exploded.

The evolution of the event in the parallel line module test was similar to what was seen in the rhombus module. Cell 6 was the first to ignite and enter thermal runaway (0 to 1740 seconds). Afterwards, the module entered the stable combustion phase, which lasted for 540 seconds. Cell 7 ignited between 2400 to 2730 seconds, which then triggered thermal runaway and flaming in Cell 5. The flame from Cell 5 was blown off by the smoke flow. The flame from Cell 7 ignited the blown off smoke and caused a jet fire. At 2721 seconds, the jet fire caused a violent ejection of black smoke from Cell 7. After 2730 seconds, flaming and smoking self-extinguished slowly. The authors report the surface and tab ignition or explosion temperature, time to ignition, maximum temperature, thermal runaway propagation time, peak HRR, and total mass loss ratio of each cell.

The surface ignition temperatures ranged from 110 to 140°C, but thermal runaway temperatures varied significantly. Huang et al. (2016) noted that it is possible that the heating effect from impinging fire accelerated thermal runaway onset. The largest mass loss percentages are correlated with peaks in HRR, ignition, and onset of thermal runaway [128].

7.1.23. Huang et al., 2020

Huang et al. (2020) explored the impact of electrical connection on thermal runaway propagation and characterized thermal runaway features of large format, Li-ion battery modules. The authors tested prismatic, 94 Ah, NMC single cells and 4-cell modules under a cone calorimeter. The single cells were tested by utilizing a 500 W heating plate placed on the sidewall of the cell to trigger thermal runaway. Cells were tested at 100% and 50% SOC. Gases were quantified via FTIR. The modules were formed by placing four batteries in a steel holder and connecting them in series, parallel, or not at all. The heating plate placed on the sidewall of one battery. Once thermal runaway was confirmed, the heating plate was removed.

The 100% single cell underwent five stages during flaming thermal runaway. In the lateral heating stage, the battery starts self-heating as the chemical components decompose and react. In the next stage, the safety valve on the cell breaks and vents jet fire and black smoke violently. Then, the jet fire and smoke decrease in the third stage. The combustible gases and ejected

electrolyte are ignited, burn, and combustion slows down as the fuel is consumed in stage four. The final stage is the end of the test.

The 50% SOC cell also had five stages of combustion. The first stage was also lateral heating; however, the other stages were different from the 100% SOC cell combustion. The cell underwent safety venting in stage two and vented jet white smoke in stage three. In stage four, the jet white smoke abated, and stage five was the end of the test. For the 50% single cell test, cell venting during thermal runaway occurred for approximately 82 seconds. The authors report the combustion characteristics of the single cell tests and total species production of toxic gases.

The module level tests had three distinct stages during thermal runaway. First, the cells are heated, which causes an increase in gas production and internal pressure. This leads to cell safety venting. In the second stage, thermal runaway has propagated to all four cells in the module and violent jet fire and black smoke are released. In stage three, the cells enter a weaker combustion stage and slowly abates as fuel is consumed. Testing revealed that thermal runaway propagates due to the heat transfer between adjacent modules. The authors noted that heat transfer through the connectors and radiation primarily drives heat transfer, while conduction through air contributes less [54].

7.1.24. Huang et al., 2021

The authors tested large format Li-ion modules with NMC and LFP cell chemistries at 100% SOC to compare their performance. Each module held four prismatic cells physically in parallel without electrical connection. The LFP cells each had a capacity of 336 Wh and weighed 2097 g. The NMC cells each had a capacity of 360 Wh and weighed 2027 g. One cell at the end of the module was heated to thermal runaway by a 0.5 kW heating plate.

Thermal runaway was defined as reaching 368°C at the front surface and 93°C at the back surface for NMC cells. For LFP cells, it was defined as reaching 335°C at the front surface and 121°C at the back surface. After reaching thermal runaway, the heating plate was turned off. Thermal runaway tests were conducted underneath a hood open to ambient air. The gases produced from the modules were analyzed for CO, CO₂, CH₄, C₂H₄, C₃H₆, H₂, HF, NH₃, and HCl using FTIR, a H₂ detector, and a HF detector. MLR and HRR were calculated using oxygen consumption, and pressure differential and smoke temperature, respectively.

The NMC modules underwent safety venting, jet fires, black smoke, and explosive into stable combustion when thermal runaway was triggered. Thermal runaway propagated through all cells in the NMC module in both NMC experiments. The NMC cells reached higher temperatures and had higher thermal runaway propagation speeds than the LFP cells. The period between safety venting and thermal runaway was shorter for NMC cells (0 to 23 seconds) compared to LFP cells (98 to 597 seconds), indicating that the safety venting did not prevent thermal runaway in the NMC modules. On the other hand, the LFP modules released white smoke when entering thermal runaway but did not achieve flaming conditions. Complete thermal runaway occurred in only one of three LFP experiments. However, the duration of thermal runaway for LFP cells (208 to 247 seconds) was longer than the duration for NMC cells (19 to 31 seconds). The time from the first LFP cell venting to the completion of thermal runaway in the last cell was a total of 2330 seconds. The time from the first NMC cell venting to the completion of thermal runaway in the last cell was a total of 838 seconds.

The peak HRR for the NMC module was 16.98 kW; however, the oxygen analyzer malfunctioned due to the deflagration. Since the LFP module did not ignite and consume oxygen, the calculated HRR was 0 kW; however, this does not reflect the energy release potential of the module. The time for propagation of thermal runaway throughout the LFP module (1715 seconds) was found to be approximately twice as long as in the NMC module (816 seconds). H₂, CH₄, C₂H₄, C₃H₆, CO, and HF were released at significantly higher concentrations in NMC modules. CO and CO₂ were the primary gases produced by both cell chemistries. The gases produced from the NMC modules had a greater peak FED¹⁰ and FEC¹¹ values (0.13 and 0.168) compared to the values for LFP (0.017 and 0.01). The LFP module was found to produce a total of 8.54 g of CO, 18.2 g of CO₂, 5.4 g of HCl, and 5.24 g of NH₃. HF was not detected during the LFP experiment. The NMC module was found to produce a total of 68.4 g of CO, 1473 g of CO₂, 1.3 g of HCl, and 2.9 g of HF. NH₃ was not detected during the LFP experiment. NH₃ was not detected in NMC thermal runaway, whereas LFP produced NH₃. There was a larger amount of ejected combustible gases per failed NMC cell (21.09 g) compared to the total ejected combustible gases per failed LFP cell (4.17 g) [55].

7.1.25. INERIS, 2022

In 2021, the French National Institute for the Industrial Environment and Risks (INERIS) performed analyzed emission factors for a variety of fuels including Li-ion batteries. FTIR was used to detect chemical compounds including CO, NO_x, acid gases, and formaldehyde. FID was used to measure VOC. In addition, metals, PCDD/F, and PAH (23 substances) were sampled and analyzed. The test results showed that for Li-ion battery fires (50% SOC) the maximum CO/CO₂ ratio¹² was 0.04, and the ratio during steady-state burning was 0.03. The maximum CO/CO₂ ratio was less than all other fuels tested, but the ratio during steady state burning was like mixed plastics. The overall VOC emission factor for Li-ion batteries was 8,420 mg/kg which was nearly equivalent to that found for oil (8,880 mg/kg). This emission factor was more than natural wood (1,500 mg/kg) and high-density polyethylene (4,200 mg/kg) but significantly less than mixed plastics (21,800 mg/kg), PVC (37,500 mg/kg), and shredded tires (54,050 mg/kg). The overall PAH emission factor for Li-ion batteries was found to be 45 mg/kg, similar to that found for crushed information technology equipment (60 mg/kg). This factor was more than those observed for natural wood (28.7 mg/kg), but significantly less than mixed plastics (1,311 mg/kg), PVC (526 mg/kg), and shredded tires (2,120 mg/kg).

Emission factors for a wide variety of other fuels were also identified by INERIS (2022). Based on these values, the Li-ion battery emission factor for HF (7 g/kg) is observed to be like the HF emission factors for electric cables (8.3 g/kg) and pesticides (9.0 g/kg) and significantly more than those for the other fuels, many of which had an emission factor of 0 g/kg. Additionally, the

¹⁰ The FED model compares the concentration of asphyxiant gases, carbon monoxide and hydrogen cyanide, against doses known to cause the effect being evaluated, e.g., incapacitation. The model assumes the impact of CO and HCN are additive and considers the impact of carbon dioxide on respiratory rate. An FED less than 1 indicates that the effect was not reached.

¹¹ The FEC model compares the concentration of irritant gases, like HF, HCl, HBr, acrolein, etc. against doses known to cause the effect being evaluated, e.g., incapacitation. The model assumes the effects of irritants is additive. An FEC less than 1 indicates that the effect was not reached.

¹² The CO/CO₂ ratio is used to evaluate combustion efficiency. A larger CO/CO₂ ratio indicates less efficient combustion and higher CO production along with higher production of other unburned hydrocarbons.

emission factor for metals from Li-ion batteries (17,000 mg/kg) and tires (60,000 mg/kg) were clear outliers from the other fuels, for which most had an emission factor of 0 mg/kg. The soot emission factor for Li-ion batteries (2.1 g/g) was also observed to be elevated compared to most other fuels.

Conversely, yields of HCN, HBr, HCl, and SO₂ were reported to be 0 g/kg for Li-ion batteries, but were produced from other common fuels such as PU (HCN = 1.8 g/kg), computer equipment (HBr = 14 g/kg), PVC (HCl = 320 g/kg), and home appliance products (SO₂ = 7 g/kg). Yields of NO_x were reported to be significantly elevated for fuels such as PU (90 g/kg), and clothes (7.2 g/kg) compared to Li-ion batteries (.9 g/kg) [87].

7.1.26. Kang et al., 2023

In an evaluation of BEV fires, Kang et al. (2023) performed independent tests on NMC battery packs extracted from the vehicle to better assess the specific contributions from the Li-ion cells. The individual cells within the battery were pouch type cells and had a capacity of 60 Ah, a nominal voltage of 3.63 V, and a mass of 887.8 g. Each module within the pack contained 27-30 cells and there were 10 modules with the pack. The complete battery pack had an energy capacity of 64.092 kWh, a mass of 449 kg, and was tested at 100% SOC. Thermal runaway was initiated via a heating sheet applied to the surface of a single cell inside the battery pack.

Tests were conducted below a conical hood connected to an exhaust duct with an airflow rate up to 3,200 m³/min. HRR and THR were calculated via oxygen consumption calorimetry. The peak HRR of the battery pack was found to be 1.54 MW and the THR was found to be 1,300 MJ. Total mass loss during the test was 28 kg. The average heat of combustion was calculated to be 45.9 MJ/kg. The authors related this heat of combustion value to typical values for polypropylene and polyethylene (44.6 MJ/kg), which typically comprise the combustible housing components of a Li-ion battery pack and typical values for separators and mixed carbonate solvents (12.7-24.7 MJ/kg) [75].

7.1.27. Larsson et al., 2016

In the study performed by Larsson et al. (2016), LFP and NCO modules were exposed to an external heat source to assess toxic gas emissions and heat release rate. HF production was measured via FTIR and in Test D, via gas-washing bottles. HF measurements using gas-washing bottles produced levels twice as high but within the same order of magnitude. The authors measured mass loss, peak HRR, THR, peak HF concentrations, total production of HF, and yields for HF by mass lost and energy capacity.

The study observed that cells with a 100% SOC produced higher peak HRRs and higher amounts of HF. It was also observed that the cell voltage breakdown appeared to occur simultaneously with HF gas emissions from the cell. Mass flow of HF was found to reach a peak value of approximately 3.0 mg/s, 1.8 mg/s, 8.0 mg/s, and 34.0 mg/s for Tests A, B, C, and D, respectively. Mass flow of HF was found to reach a peak 1-minute average value of approximately 2.4 mg/s and 1.1 mg/s for Tests A and B respectively; 1-minute averages of HF mass flow were not reported for Tests C and D [68].

7.1.28. Larsson et al., 2017

In the analysis performed by Larsson et al. (2017), it was identified that LiPF_6 and other lithium salts containing fluorine are found in the electrolyte of typical Li-ion batteries. These fluorine-containing electrolytes can vaporize and be vented from Li-ion battery cells during an overheating event such as a fire or thermal runaway. In such an event, the fluorine in the electrolyte, or in other components (i.e., PVdF binders in the electrodes, flame retardants in separators, and fluorophosphates in electrode materials), can be released as HF, PF_5 , and/or POF_3 . It was also noted that the decomposition of LiPF_6 can be accelerated in the presence of water.

The analysis included experimental testing of seven different types of Li-ion batteries exposed to an external heat source which led to ignition of the battery cells. Tests within the same battery type were also conducted with various SOC. It was observed that the HRR only experienced distinct peaks when the cells were at a 100% SOC. At lower SOC, the HRR curves were relatively smooth. The peaks in the 100% SOC tests were attributed to the violent venting of cells which led to ignition of emitted gas and intense flares. While there were significant differences in the peak HRR for cells at a different SOC, the THR normalized by capacity in Wh varied little. The peak amount of HF produced was also highly dependent on the SOC, however the total amount of HF produced normalized by capacity was mostly dependent on the cell type, not the SOC.

HF was measured by FTIR and gas-washing bottles. Generally, the gas-washing bottles measured higher levels of HF, however, trends were similar across both detection methods. Pouch type cells were found to produce the highest levels of HF; this was hypothesized that this was due to cylindrical and prismatic cells requiring a higher pressure in order to vent, thus resulting in a more rapid release of electrolyte vapors and a less complete burning of these vapors. The authors report the HRR and HF production measured during the 100% SOC tests. Production of POF_3 could only be detected in two tests of Type A batteries at 0% SOC. The normalized total yield of POF_3 from these two tests was calculated to be 15 to 22 mg/Wh. The effect of the application of water mist on the production of HF was also assessed in the series of tests. Water application temporarily increased the rate of release of HF but did not have a significant impact on the total amount of HF released [69].

7.1.29. Lecocq et al., 2016

Single-cell tests were conducted on pouch, LFP cells with a capacity of 1.3 Ah/4.2 Wh and a mass of 38 g. Tests were performed with either LiPF_6 or LiFSI electrolyte to see if electrolyte composition influenced gas emissions, HRR, and/or MLR. The cells were charged to 0, 50, or 100% SOC. The pouch cells were ignited using the Tewarson apparatus radiating a 25 kW/m^2 heat flux and a pilot flame. A hood was utilized for gas collection. Samples were analyzed for CO, CH_2O , HCN, NO_x , SO_2 , HF, and fluorinated species using FTIR.

The LiFSI electrolyte cells had an abrupt heat release at 50 and 100% SOC, unlike the LiPF_6 electrolyte cells. The authors proposed that the rapid release may be due to the sudden and highly exothermic redox process between the electrode and LiFSI. The exothermic process could cause the electrolyte to evaporate rapidly, resulting in rapid combustion. At 0% SOC, neither electrolyte had a significantly rapid reaction. The shorter peak at 0% SOC for the LiFSI electrolyte cells indicates that it might be more reactive than LiPF_6 . The total gas production for HF, CO, and SO_2 is reported in the original paper. The production of HF tended to decrease with SOC for LiPF_6 . Lecocq et al. (2016) proposed that either a) certain formation processes are dominant during

flaming, or b) cells at a lower SOC have a longer fire duration and could maintain the decomposition temperature required for HF production longer. The production of HF in LiPF_6 is a magnitude greater than production in LiFSI. The authors noted that this difference could be due to LiPF_6 thermally decomposing into gaseous PF_5 rapidly. They reasoned that gaseous PF_5 is very reactive and can easily diffuse outside the cell to form HF. On the other hand, LiFSI does not decompose into a gas and release fluorine. Only LiFSI produced SO_2 , decomposition may take place inside the cell which may favor formation of Li_2SO_4 [129].

7.1.30. Lee & Stoliarov, 2018

Lee and Stoliarov (2018) performed testing on various arrays of cylindrical LCO cells to better understand dynamics, energetics, and gaseous emissions of Li-ion battery pack failures. The individual cells had a capacity of 2.6 Ah, a nominal voltage of 3.7V, and a mass (without packaging) of 43.57 g. At 100% SOC, the average stored electrical energy was calculated to be 34.1 kJ.

A series of tests were performed to assess the amount of heat generated chemically from the reactions between the battery cell components during non-flaming thermal runaway, as well as heat generated during flaming thermal runaway. The tests showed that, during non-flaming thermal runaway, at 100% SOC, approximately 59 kJ of heat was generated per failed cell, i.e., 1.73 kJ of heat generated per kJ of stored electrical energy. Meanwhile, the tests showed that heat generated from flaming thermal runaway of the cells was approximately 63 kJ; these results represented fire conditions that were under-ventilated. For well-ventilated conditions, values of 107 kJ/cell and 3.35 kJ/ kJ stored electrical energy were achieved.

The dynamics of thermal runaway within the cell arrays was also studied. Generally, it was found that a cell went into thermal runaway when, at least, one adjacent cell had undergone thermal runaway. While the propagation trends were similar throughout the tests, timing of cell failure was found to be considerably varied, despite well-controlled conditions [130].

7.1.31. Liu et al., 2020

The authors induced thermal runaway in Li-ion batteries to characterize combustion and fire behavior, as well as gas release. The cells used were prismatic LFP Li-ion batteries with LiPF_6 electrolyte. The cells had a capacity of 22 Ah and a nominal voltage of 3.2V. The cells were tested at 0, 50, 75, and 100% SOC. Cells were placed under a hood for gas sampling. A Servomex 4100 analyzer was utilized to determine O_2 , CO_2 , and CO concentrations. A semiconductor gas sensor was utilized for H_2 , and an optical gas sensor was utilized for HF. Thermal runaway was initiated using a 500 W heating plate wrapped around the surface of the cell. Piloted ignition was used to ignite combustible gases. The HRR contribution from the igniter was subtracted from total HRR to isolate the contribution from the cells. Thermocouples were placed on the cell surface, tabs and above the safety valve to measure temperature. The 75% SOC cell was only analyzed for HRR and THR.

The authors divided flaming thermal runaway into three stages: venting, ignition and combustion, and extinguishment or jet flow. Combustion was initially stable, then thermal runaway triggered jet fire for the higher SOC cells. No jet fire or thermal runaway were observed for the 0% SOC cell. The authors found that the 100% SOC cells vented within a shorter period of

time compared to the 0 and 50% SOC cells. The flaming period for the cells at 100% SOC was shorter compared to flaming period for 0 and 50%. Additionally, the 100% SOC cell had more violent jet fire and jet flow during extinguishment compared to the 50% SOC cell. The higher SOC cells ejected a larger quantity of cell contents, including electrolyte, generated gases, and materials from the separator, electrode, and binders.

The authors reported the peak HRR and THR of the cell for each SOC. The HRR values for the 100% SOC cells are smaller than those for the 50% SOC cells due to the significant smoke generation during the jet fire and the jet flow. The 75% SOC cells had the highest peak HRR and THR.

CO production tended to increase with SOC, which indicated that combustion efficiency decreased with SOC. The authors attributed this trend to the longer stable combustion time in lower SOC cells, violent ejection of cell contents in higher SOC cells, and the reduction of CO₂ with Li_xC₆ for higher SOC cells. H₂ production was attributed to reactions between the PvDF binder and Li_xC₆ and only occurred in the 100% SOC cell test. Total HF released was significantly higher for 100% SOC cells. Additionally, the amount of HF absorbed into battery components is less for 100% SOC cells. The 100% SOC cells released larger quantities of HF due to the larger amounts of electrolyte bursting and the higher venting pressure. The authors note that HF may have lost reactivity through interactions with NH₃ and the reported values give the lowest HF production [70].

7.1.32. Liu et al., 2021

Liu et al. (2021) performed testing on commercial LFP Li-ion batteries to assess thermal runaway behavior and the toxicity of vented gases. The batteries utilized in the tests consisted of two LFP pouch cells connected in parallel. The total nominal capacity of the battery was 243 Ah/778 Wh. The batteries were tested at 0, 50, and 100% SOC. Two cases of tests were conducted. In Case 1, an igniter at the safety valve opening was used to ignite the vent gases. In Case 2, no igniter was used, and no flaming ignition occurred. Thermal runaway was initiated via an electric heating plate and a ceramic fiber blanket enwrapped the battery and heater. Tests were conducted within a combustion chamber and products of combustion were captured via an exhaust hood and a sampling duct. Oxygen, carbon monoxide, and carbon dioxide were quantified online via a gas analyzer and HRR was determined based on these measurements and the method of oxygen consumption. Additional gases were analyzed with FTIR.

In Case 1, the cells underwent four stages of behavior during the tests. In stage 1, the safety valve opened and vented gases, which subsequently ignited and caused deflagration. In stage 2, the flame reduced in size and continued to burn in a steady state. In stage 3, a vertical jet flame occurred, however cells at 0% SOC did not experience the jet flame stage. In stage 4, the flames decreased until extinguishment.

In Case 2, the batteries released an initial jet flow of gas, but this release was of short duration. The batteries then experienced a stable state at which small amounts of smoke were emitted, with a downward behavior. The authors determined the gases released during these initial stages were electrolytes. The batteries then experienced a violent venting stage, which in the 100% SOC tests, ejected solid materials as well. Cells at 0% SOC did not exhibit the violent venting stage. After the major venting event, emissions decreased and eventually ceased. The authors noted that for flaming conditions, when compared to non-flaming conditions, the time from initial venting to the

onset of thermal runaway during is decreased by 23% in the 50% SOC cases and 37% in the 100% SOC cases. The authors presented data on thermal runaway onset temperature, peak HRR, THR, effective heat of combustion, total mass loss, and peak MLR. The effective heat of combustion was calculated as an average based on the THR and the total mass loss. The authors noted that the THR increased with increasing SOC but that the heat of combustion remained relatively constant.

The authors reported results from the Case 1 tests regarding total vent gas production for CO, CO₂, HF, NO, HCl, NH₃, and SO₂. Gas production quantities were not reported for Case 2 (non-flaming) tests [71].

7.1.33. Long et al., 2013

In cooperation with the FPRF, Exponent, Inc. assessed the best practices for emergency response to electrical vehicle fires involving Li-ion batteries, of unknown chemistry. The analysis included full-scale fire testing of electrical vehicles which incorporated suppression methods. Two types of tests were performed: 1) a free-burn of a standalone Li-ion battery pack without suppression, and 2) burns of Li-ion battery packs mounted within a vehicle with suppression.

The standalone battery test was conducted using a propane burner. The external heat source was used to induce the cells of “Battery B” into thermal runaway. Battery B was a 16 kWh, t-shaped battery pack enclosed in a fiberglass case. The test results showed that when the external heat source was active, there was a visible release and ignition of electrolyte material. When the external heat source was removed (at approximately 20 minutes), the fire intensity decreased and was observed to resemble a controlled release of flammable gases.

The peak HRR was measured to be 698 kW at 17 minutes and 33 seconds. However, the propane burners were active at this time and estimated to contribute 400 kW to the HRR. Therefore, the peak HRR of the flaming thermal runaway condition was estimated to be 300 kW. The average HRR for the duration of the test was 128 kW, and the total heat released was 720 MJ. During the test, air samples from a truncated cone hood above the burning battery were collected via Tedlar grab bags every 5 minutes, with each sample pulled over a 1-minute period. The samples were analyzed for the following gases using FTIR: HCl, HF, HBr, HCN, CO₂, CO, NO_x, SO₂, acrolein, and formaldehyde. Only CO and CO₂ were detected; measurement values were not reported.

Six full-scale fire and suppression tests were performed with Li-ion battery packs mounted in a vehicle. Three tests were performed utilizing “Battery A”, and three tests were performed utilizing “Battery B.” Battery A was a 4.4 kWh, rectangular battery pack enclosed in a metal case. Battery B was the same as used in the standalone battery test previously discussed. Further details on the cell type, configuration, and chemistry were not provided in the analysis report. For each battery type, two tests were performed with only the battery mounted within the vehicle, and one test was performed with additional interior finishes in place in the vehicle, such as seats, carpeting, and a dashboard. HRRs and products of combustion were not measured for the full-scale vehicle fire and suppression tests. However, for the Battery A and Battery B tests with the vehicle interior finishes in place (Tests A3 and B3), water samples from extinguishment were collected. At the conclusion of these two tests, after suppression had ceased, one pint of water was collected off the ground two feet in front of the vehicle and was later chemically analyzed in a lab. The water samples were first filtered to remove particulates and then analyzed for pH, cations, anions, and organic and inorganic carbon. These results were presented in the original paper.

A lower pH and elevated levels of chloride and fluoride were observed in the collected water from suppression activities in both tests. Due to the understanding that HF and HCl will dissociate into cations and anions in an aqueous solution and that hydrogen cations cause a decrease in pH, the analysis concluded that HF and HCl were likely present during suppression. The presence of HF and HCl was attributed to the thermal degradation of polymers contained in the batteries, as well as thermal decomposition of the battery electrolytes [111].

7.1.34. Lopez et al., 2015

Cylindrical and prismatic LCO cells were tested to determine if geometry, spacing, connection method, and insulation influenced thermal runaway behavior. The cylindrical cells were 18650 cells, 2.8 Ah capacity equipped with side vents. The prismatic cells had a capacity of 5.3 Ah and were equipped with a header vent.

One cell in each module was forced into thermal runaway via film heaters. For the 9-cell modules, cell 9 at the center was the initiating cell; Cell 4 was the initiating cell for the 4-cell module. The film heaters were shut off after the initiating cell went into thermal runaway. Thermal runaway was defined as a surface temperature exceeding 200°C. The initiating cell had a 1 A current and 20V applied to it. Surface temperature and open circuit voltage (OCV) were measured to characterize thermal runaway.

The cylindrical cells adjacent to and/or electrically connected to the initiating cell had overall higher temperatures and lower OCVs. There was excessive smoke and high temperatures, but no flaming, rupture, or thermal runaway propagation. At closer spacings (1 to 2 mm), there was more char and melting plastic on the cells near the trigger cell. The average and maximum temperatures of adjacent cells were higher at closer spacings. Directly adjacent cells suffered more damage than diagonal cells. The cells connected by serpentine tabs had higher maximum temperatures and a larger decrease in open circuit voltage.

The wider spacing in the prismatic modules did not prevent thermal runaway propagation or temperature increase due to the side vents releasing hot gases that heated up surrounding cells. Measurements showed that the surrounding cells were heated over 600°C, indicating that they also underwent thermal runaway. All cells in the 9-cell prismatic modules read 0 OCV except cells 1 and 9. With the addition of insulation, the trigger cell was able to eject without affecting the other cells. Unlike the uninsulated modules, no evidence of venting or burned tabs was found. Temperature rise was not sustained, and the cells had higher OCVs at the end of the test.

For the prismatic modules at 50% SOC, no flaming was visible, unlike 100% SOC modules. There were no sustained high temperatures or venting in cells aside from the initiating cell. Three out of the four cells had low OCVs. However, there was still significant charring and melting at initiating cell [131].

7.1.35. Mayonado et al., 2024

To evaluate the effectiveness of UL 9540A test standard data for predicting thermal runaway propagation and associated hazards, Jensen Hughes, Inc. conducted a meta-analysis of data from publicly available UL 9540A tests. Mayonado et al. (2024) found that protocol in UL 9540A tends to give the lab at which testing is conducted discretion on where and how to initiate thermal runaway, as well as the number of cells that are forced into thermal runaway to assess propagation.

There was a larger percentage of failed cells in the module level tests compared to their respective unit level tests. The authors noted that this discrepancy may have been caused by the lower percentage of cells forced into thermal runaway during unit level testing compared to module level testing. Additionally, the authors found that a majority of UL 9540A tests reported a peak HRR of 0 kW. The authors noted that during thermal runaway, heat is generated by rapid electrical discharge, the decomposition of the cell contents, and the hot gases released. However, oxygen consumption calorimetry does not capture these sources of heat and are more suited to combustible fires. The authors concluded that the 0-kW peak HRR measurements underestimate the heat release potential of Li-ion cells. The authors reported the results of the meta-analysis for LFP and NMC cell level tests. Data reporting a peak HRR or THR of 0 was excluded.

The authors noted that heat release behavior is significantly influenced by cell chemistry and cell geometry and that measured peak heat release rates can vary greatly depending on the measurement technology used. They also noted that cell level UL 9540A data tends to predict higher peak HRR normalized by electrical energy and lower total heat released normalized by electrical energy, when compared to results from Ditch & Zeng (2020) which evaluated a full-scale unit [13]. Based on this, for full scale Li-ion battery peak heat release rate bounding, Mayonado et al. (2024), estimated a peak HRR of 0.2 kW/Wh. In looking at the gas production data, the authors observed that total gas quantities also vary greatly by cell chemistry and cell geometry and may also be influenced by failure modes and test instruments [12].

7.1.36. Meng et al., 2020

Meng et al. (2020) investigated the correlation between SOC and combustion behavior and toxicity in LFP Li-ion cells undergoing thermal runaway. The cells utilized in the test were 22 Ah/81 Wh, prismatic LFP cells charged to 0, 50, and 100% SOC. Thermal runaway was initiated via an electric heater attached to one side of the battery. The battery and heater were enwrapped with a noncombustible aluminum silicate insulation to prevent heat loss to the environment. An igniter was utilized to ignite the vent gases as they were released from the cell. The tests were conducted in a combustion chamber equipped with a collection hood and exhaust system. Gas was sampled from the exhaust duct and an oxygen analyzer was used to determine concentrations of oxygen, CO, and CO₂. HRR was determined using the oxygen consumption method. HF concentrations were determined via a gas analyzer with an optical gas sensor for HF.

In the 100% SOC and 50% SOC tests, as the cells were heated, they began to expand due to production of gases within the cell from the reaction of electrolyte and electrode materials. The internal pressure continued to increase until the safety valve opened, emitting white electrolyte and other combustible gases. These gases were ignited by the manual igniter and a stable stage of combustion occurred as gases continued to be emitted. The cells then underwent a stage of reduced combustion intensity, followed by a violent ejection of cathode and anode materials and a large amount of electrolyte and other gases, creating a vertical jet fire. Another stable combustion stage continued until the fire started to decay and eventually extinguished.

It was found that 50% SOC cells took longer to vent and enter thermal runaway, with an overall longer period of combustion. The 0% SOC cells only experienced one stage of stable combustion and no jet fire. In the 100% SOC test, which experienced the highest temperatures, the maximum surface temperature of the cell was 451°C and the maximum flame temperature was 943°C, at 5 cm above the safety valve.

Results regarding peak HRR, THR, total gas production, and species gas production rate were reported in the original paper. The authors noted that the production of HF increased with increasing SOC, with regards to both total production and peak production rate. Total CO₂ production increased with decreasing SOC, but the peak production rate was highest in the 50 and 100% SOC tests. Total CO production and peak CO production rate were highest in the 50% SOC test [72].

7.1.37. Nedjalkov et al., 2016

Li-ion cells were tested in three different scenarios by Nedjalkov et al. (2016) to assess the toxic gas emissions from damaged Li-ion batteries. Slightly overcharged (4.3V), pouch NMC cells, with a capacity of 40 Ah were used in all tests. The cells had graphite anodes, and the electrolyte composition was EMC and EC with LiPF₆ salt. During the tests, emission gases were pumped to analyzers. GC-MS was used to detect EMC, DEC, EC, benzene, toluene, styrene, and biphenyl. Quadruple MS was used to detect benzene, toluene, acrolein, CO, and CO₂. Ion chromatography was used to detect HF.

The three test scenarios included (1) cell catching fire, (2) no combustion of cell, and (3) no combustion of cell and gas filtration. In all three scenarios, the cell was in a barrel and punctured with a nail to induce thermal runaway. In Test Scenario 1, the barrel cover was partly shut to prevent the barrel from exploding and to retain most of the emission gases. HF, CO, and CO₂ were not measured in this test scenario. In Test Scenario 2, the cell was wrapped in a gas-permeable, textile composite structure to prevent flaming conditions. Test Scenario 3 was run in the same manner as Test Scenario 2 except that a gas filtration unit was mounted on top of the barrel and all gas emissions were collected after filtration. The filter consisted of five levels; a coarse particulate separator, activated charcoal, potassium permanganate, activated alumina, and a fine particulate filter. It was found that Scenario 2, i.e., no flaming conditions or filtration, produced the highest concentrations for each gas. In each test, the total volume of vent gases produced from the cell was approximately 200 liters.

It was reasoned that the flaming thermal runaway of the cell in Scenario 1 produced less toxic gas emissions because the reaction of the organic compounds with oxygen produced CO₂ and H₂O. However, only a portion of the VOC released from the cell were combusted due to the sudden venting of the cell causing the displacement of atmospheric air within the barrel; this reduction in available oxygen prevented complete oxidation of all components, and instead, these compounds, mainly consisting of the electrolyte's chemistry of EMC and EC, were exhausted. Traces of DEC, benzene, toluene, styrene, and biphenyl were detected. In Scenario 2, almost no oxidation took place, and therefore, a larger amount of unburned organic substance was exhausted. There were 155 different constituents detected in Scenario 2. It was reasoned that this variety, along with the higher concentrations of the gases, was due to the thermal decomposition of EMC electrolyte. The EMC was thought to be decomposed into free ethyl and methyl radicals, as well as free vinyl and ethylene radicals. These radicals can lead to the formation of various VOC and PAH. HF was not measured in the flaming thermal runaway scenario. HF was measured in Scenario 2 and found to be 1,640 ppm. Production of HF was attributed to the decomposition of the LiPF₆ salt in the electrolyte [66].

7.1.38. Peng et al., 2020

Peng et al. (2020) studied the release of toxic gases from thermally induced failure of Li-ion battery cells. In their tests, thermal runaway of a single 68 Ah pouch cell was induced via an external heater. The cells had a nominal voltage of 3.22V, an initial mass of approximately 1250 g, and LiFePO₄/graphite electrodes. Tests were run with the cells at 0, 50, 75, and 100% SOC. The tests were conducted in a well-ventilated chamber, and gas samples were extracted from the exhaust stream and analyzed for toxic gases via FTIR. An electric spark igniter was placed near the bottom of the battery to ignite vented flammable gases.

The tests showed that, regardless of SOC, the cells exhibited common burning behaviors, separated into the following five stages:

1. Heating and expansion- At this stage, the cells are being heated externally. The surface of the cells shows slow expansion due to an increase of pressure inside the cell caused by the accumulation of thermal decomposition gases. Eventually, some flammable gases are vented and ignited by the electric spark igniter.
2. Stable combustion with small flame- At this stage, the vented gases from the cell are burning in a small, stable fire.
3. Jet fire- During this stage, the fire is initiated when the separator in the cell fails causing thermal runaway. A significant release of gases results in a high-speed, jet flame.
4. Second stable combustion- At this stage, the combustion returns to being stable, though larger than the Stage 2 combustion.
5. Abatement and extinguishment- At this stage, the fire decays until extinguishment.

It was observed that cells with a larger SOC had a longer and more violent jet flame in Stage 3, and a larger fire at Stage 4. HRR was also measured during each test, and cells with a higher SOC had a higher peak HRR. The heat release rate per unit area (HRRPUA) was derived from these results and calculated to be 2.1 MW/m² for the cells at 100% SOC. The cells at 100% SOC produced the highest THR value. THR results for each SOC are presented in the original paper, along with peak HRR and ignition times. The authors also reported the peak species gas concentrations at various SOC. CO production was measured during the tests, and the peak CO concentration was 258 ppm produced at 100% SOC. HF, SO₂, NO, NO₂, NO, and HCl were also analyzed during the test using FTIR. Only the peak concentration of HF (165 mg/m³) was found to exceed the IDLH limit (24.6 mg/m³). This measurement was taken in the exhaust stream close to the source.

HF production was attributed to electrolyte (LiPF₆), the PVdF binder, and possibly coating materials, such as AlF₃. SO₂ production was attributed to sulfur-based compounds used as reduction-type additives. NO and NO₂ are considered reaction products, and HCl production was attributed to flame-retardant additives in the plastic packaging of the cell.

In connection with the experimental tests, Peng et al. (2020) performed a toxicity analysis using the methods outlined in ISO 13571. The authors concluded that the effects of irritant gases are more significant than the effects of asphyxiant gases (CO and CO₂) although neither FED reached unity, i.e., the evaluated effect. He also concluded that HF and SO₂ would be more impactful than NO_x and HCl [73].

7.1.39. Premnath et al., 2022

To characterize the particle emissions produced by Li-ion battery thermal runaway events, Premnath et al. (2022) forced LFP and NMC modules into thermal runaway. The LFP modules contained 96 cylindrical cells, with a cell capacity of 8.28 Wh and a cell mass of 70 g. The NMC modules contained 30 pouch cells, with a cell capacity of 249 Wh and a cell mass of 820 g. Two LFP modules and the NMC module had thermal runaway initiated by nail penetration, and two LFP modules underwent overcharge.

An open-air calorimeter was used to sample gases. Two engine exhaust particle sizers (EEPS) were used to measure particles between 5.6 to 560 nm. One unit was coupled with a solid particle sampling system to measure solid particle number concentration and size distribution. The other EEPS measured both solid and volatile components. A micro-soot sensor (MSS) with detection limits of 5 $\mu\text{g}/\text{m}^3$ and 50 mg/m^3 measured black carbon concentration. The EEPSs and MSS both took measurements in real time. Gravimetric filters measured PM_{2.5} and were also sublimated to determine the volatile components. Organic carbon/elemental carbon analysis was performed on samples captured by filters. Concentrations of CO₂, CO, CH₂O, NO, NO₂, HCl, HF, HCN, CH₄, and C₃H₈ were measured by FTIR. The authors reported a summary of measurements for all tests.

The LFP modules undergoing nail penetration produced visible smoke and flames. For Test 1, the fire lasted for one minute and self-extinguished. Test 2 only produced a small flame. Thermal runaway did not propagate to other cells. There were no significant peaks in gas production for Test 1, whereas Test 2 had peaks in alkyl carbonate compounds.

The LFP overcharge tests had more dramatic thermal runaway events compared to the nail penetration tests. Test 3 underwent smoke venting at 16 min after overcharging. Sparks appeared at 17 min 21 s, and the entire module caught fire, destroying the module. Similar events occurred in Test 4. There were significant peaks in CO₂, CO, and hydrocarbons. Peak HF concentration was measured at 177 ppm for Test 3. Test 4 produced similar concentrations for all gases.

Unlike the LFP nail penetration tests, the NMC module caught fire within seconds and thermal propagation spread throughout the module. By the end of the test, the entire module was destroyed. FTIR shows intense peaks in CO₂, CO, CH₂O, and NO during thermal runaway. HF was not observed in the NMC test and the authors contributed this to the lack of fluoride in the anion salt used in the cells.

Premnath et al. (2022) concluded that the initiation of thermal runaway (nail penetration vs overcharge), the cell chemistry, physical dimensions, and arrangement of cells in the module could influence emission characteristics. The HF concentrations for the LFP overcharge tests exceeded the IDLH threshold, i.e., 30 ppm, and the formaldehyde concentration for NMC nail penetration test exceeded the IDLH threshold, i.e., 20 ppm [88].

7.1.40. Quant et al., 2023

Testing was performed on BEVs and compared to internal combustion engine vehicles (ICEV) data. Quant et al. (2023) conducted fire tests on one BEV, one BEV with the battery pack removed, and one battery pack from a BEV. The ICEV was filled with 20 L of petrol (half-tank), and the remaining 20 L was poured in a tank below the vehicle. The battery pack contained 18 modules (216 cells) with NMC chemistry and had a 50-kWh capacity. It was charged to 90% SOC.

The BEV without a battery and the ICEV were heated by a 30 kW propane gas burner placed below the engine compartments. The full BEV and battery pack were heated below the rear of the battery pack. For the battery pack, the burner HRR was increased to 70 kW after 60 min due to no thermal runaway. The 70 kW HRR immediately triggered thermal runaway after which the burner was lowered to 30 kW. The battery pack was shielded to mimic the protection of the chassis. The ICEV, full BEV, and battery pack fires were suppressed using an overhead sprinkler system supplied by tap water. The suppression system was activated when HRR reached 1 MW for the vehicles and after 30s of visual detection of thermal runaway for the battery (342 kW). The battery pack was flushed after the fire test ended, since it was shielded during the test. The BEV without a battery was allowed to burn freely. The HRR and fire behavior was recorded. A hood collected the smoke and gases generated, which were analyzed for PAH. The ICEV produced 8 g of PAH. The BEV without a battery produced 9.5 g of PAH, whereas the full BEV produced 5 g and the battery pack produced 3 g of PAH. Acenaphthylene, acenaphthene, and dibenz[a,h]anthracene were not found in any of the emissions.

For the ICEV, the suppression was pre-set to run for 30 minutes. The full BEV was also set to the same duration, but the suppression was turned off after 10 minutes to prevent the system from extinguishing. After 15 minutes, the suppression system was turned back on for an additional 20 minutes. Water was applied to the battery pack for 20 minutes. Approximately 10,800 liters of water were applied via the suppression system. The first peak in HRR for the BEV without a battery was due to the engine compartment, which made up 28% of the THR. The second peak was caused by the rear of the vehicle becoming involved in the fire. The THR for the BEV without a battery was 5 GJ. The first peak in HRR for the ICEV was due to the petrol burning (26% THR), and the second peak was due to involvement of the passenger compartment. The THR for the ICEV was 6.1 GJ. For the full BEV, the rear window ruptured during the first peak, which may have helped decrease HRR. The first two peaks in HRR occurred while suppression was active, while the third peak was not suppressed. The third peak contributed 73% to the THR. The full BEV's THR was 5.7 GJ. The THR of the battery pack was 0.8 GJ and flaming lasted for 20 minutes.

The runoff firewater was collected and analyzed for inorganics, VOC, PFAS, and acute toxicity. Mercury, cadmium, and arsenic were not found in any of the tests. Antimony ranged from 40 to 240 µg/L for all tests. The BEV without a battery produced the largest amount of total soot (10 kg) and had a concentration of 30 µg/L copper. The ICEV produced a total soot of 6.5 kg and had concentrations of lead at 65 µg/L, copper at 90 µg/L, VOC at 2600 µg/L, and total PAH at 12.5 µg/L. It had the largest copper concentration out of all the tests. The BEV produced 5.2 kg of soot and had concentrations of copper at 9 µg/L, lithium at 30 mg/L, and total PAH at 2.6 µg/L. It is possible that the ICEV and BEV had a lower total soot amount due to the soot being washed away. The battery pack had concentrations of lithium at 110 mg/L and PFAS at 4800 µg/L. Boron and aluminum were also present in the battery pack firewater. The battery was flushed after the test, which may have increased the amount of PFAS and heavy metals released. It is unknown which components of the battery released the PFAS and heavy metals. Chloride ranged from 110-1300 mg/L for the vehicles compared to 35 to 50 mg/L for the battery pack. The BEV without battery and ICEV had fluoride ranges of 2 to 8 mg/L compared to 20 mg/L for the full BEV and 70 mg/L for the battery pack. There were six different PAH found for ICEV compared to two different PAH for full BEV, and no PAH in the battery pack test. VOC and PAH were not detected in the extinguishing water for the battery-only tests.

The firewater runoff toxicity was evaluated through pH, salinity, conductivity, and acute toxicity criteria for microorganisms. An EC_{50} below 20 %vol was considered high toxicity, and an EC_{50} of 20 to 70 %vol was considered intermediate toxicity. The EPA suggests a pH of 6.5 to 9.0 for freshwater. A pH level below 5, as was found in the ICEV fire water runoff, is likely to be lethal to many stream species. The values highlighted in red are considered "high toxicity", and the values highlighted in yellow are considered "intermediate toxicity".

Firewater samples were also analyzed for metals, ions, VOC, PAH, and PFAS. Mercury, cadmium, and arsenic were not found in any of the samples. Lead was only found in the water from the ICEV test, and copper was found in the highest concentration from this test as well. Antimony concentrations were found to be higher in the ICEV and BEV test compared to the battery only test. Lithium, manganese, nickel, and cobalt, which are all metals commonly used in Li-ion batteries, were found to be higher in the BEV and battery only test when compared to the ICEV test [76].

7.1.41. Sturk et al., 2015

Sturk et al. (2015) tested LFP and NMC pouch cells individually and in 5- or 10-cell modules to investigate the effects of abuse conditions. Modules were tested with physical connection only or with electrical and physical connection to assess if the electrical connection influenced thermal runaway behavior. The cells were charged to 25, 50, 75, or 100% SOC. Some cells were also completely discharged and short-circuited to produce 0V cells. HRR was quantified by oxygen consumption calorimetry. Total HF production was quantified by a combination of FTIR, ventilation filters analyzed for fluorine post-test, and gas wash bottles.

While SOC tended to increase HRR for LFP cells, it appears that the activating effect of SOC rapidly dropped. There was no significant difference between the HRR for 50 and 75% SOC LFP cells. At 75 and 100% SOC, NMC cells showed a more rapid HRR onset and a rapid decrease in HRR. The cells with lower SOC had lower peak HRRs and a sustained curve. The peak HRR and for NMC cells was significantly greater than LFP cells. The higher HRR rates could be due to the higher reactivity in the NMC chemistry. The number of cells tended to increase the overall peak HRR; however, the contribution per cell decreased significantly. The modules at 100% SOC had a higher peak HRR compared to 0V.

The total energy released per cell remained relatively similar between LFP and NMC cells, for all SOC. However, due to the higher capacity of the NMC cells, the energy released per Ah capacity was significantly higher for the LFP cells. The total heat generated determined from tests of each cell chemistry at various SOC is provided in the original paper.

The NMC cells released significantly less HF than the LFP cells. For both cell chemistries, SOC tended to increase the total HF production; however, the total HF produced for the pouch cells at 0V was comparable to HF production at 75 or 100% SOC. The total HF generated per cell is reported in the original paper.

An additional test (Test C) on an E-vehicle battery pack was conducted. The battery contained 200 NMC cells within 10 modules. The total pack voltage was 402V, and it was tested at 80% SOC. The NMC battery pack generated an HRR of 0.5 MW. No fluorinated compounds, including HF, were detected by FTIR. The authors did not offer an explanation as to why the battery pack produced no HF, whereas the NMC pouch cells still produced HF. The flames were extinguished

with water. While the battery did not reignite, it continued producing gases and maintained an internal temperature of 300 to 350°C for hours after quenching. Sturk et al. (2015) concluded that cell level test data on HF emissions and heat release rate cannot be easily extrapolated to multicell assemblies [74].

7.1.42. Sturk et al., 2019

Testing on two types of Li-ion pouch cells, LFP and NMC/LMO, was performed by Sturk et al. (2019) to assess the gases formed under heating conditions without ignition. The LFP cells had a rated capacity of 7 Ah and were charged to 3.3V and the NMC cells had a rated capacity of 14 Ah and were charged to 4.1V. The LFP cells each weighed 236 g and the NMC cells each weighed 385 g. In each test, five cells at 100% SOC were clamped together and placed on a heating plate. The heating plate induced thermal runaway of the bottom cell, which then propagated upwards through the other four cells. HF, as well as other gases of interest, were detected via FTIR and gas wash bottles.

The test results showed that the LFP cells produced a total gas volume of 50 L (42 L/kg of battery) over an event duration of approximately 45 minutes while the NMC/LMO cells produced a total gas volume of 1500 L (780 L/kg of battery) over an event duration of approximately 4 minutes. The venting times of the LFP cells were observed to be approximately 10 times longer than the NMC/LMO cells. The total amount of HF measured via FTIR was 1.8 g (1.5 g/kg battery) for the LFP cells and 1.7 g (0.9 g/kg battery) for the NMC/LMO cells. The total amount of HF measured via wash bottles was 4.2 g (3.6 g/kg battery) for the LFP cells and 6.5 g (3.4 g/kg battery) for the NMC/LMO cells. While the total amounts for the two cells reported by FTIR are nearly equivalent, when normalized to the cell energy, the LFP had a significantly higher yield of 16 g/kWh compared to 6.0 g/kWh for the NMC/LMO cells. Sturk et al. (2019) concluded that these results indicate that LiPF_6 quantities are not necessarily proportional to battery weight and therefore, total production of HF can be hard to predict based on battery weight alone. It was also identified that the test results suggest that extended duration of a thermal event favors the production of HF. Other gases detected via FTIR included DEC, DMC, EMC, and PC. POF_3 could not be conclusively identified for either of the cell types. Additional VOC were identified using GC-MS and FID was utilized for benzene and toluene for the NMC/LMO cells [8].

7.1.43. Wang et al., 2020

To assess potential soil pollution due to heavy metals dispersed into the air during a thermal runaway event of Li-ion batteries, Wang et al. (2020) performed a follow up analysis to Zhang et al. (2019a) [81] and Zhang et al. (2019b) [86] using the same experimental set up. A 900g, 50 Ah, 3.65 V, NMC, prismatic Li-ion cell at 100% SOC was forced into thermal runaway via an external heater. The anode material was mainly graphite. The cathode current collector was aluminum foil, and the anode current collector was copper foil. The shell material of the cell was an aluminum alloy. The test was conducted within an inert chamber and all PM that settled within the chamber was collected after termination of the thermal runaway event. The PM was separated into 3 samples by size, 0 to 50 μm , 50 to 100 μm , and 100 to 500 μm . These samples were analyzed for Ni, Cu, Zn, and Cr content via ICP-MS. The total mass of all PM collected was 14.57 g, accounting for 1.6% of the total cell mass prior to thermal runaway. Of the PM collected, 0.005% were 0 to 30 μm , 8.48% were 30 to 50 μm , 41.29% were 50 to 100 μm , 34.46% were 100 to 250 μm , and

15.77% were 250 to 500 μm . Wang et al. (2020) concluded that Li-ion batteries have the potential to contaminate soil and water through the transport of Ni, Cu, Zn, and Cr in PM [84].

7.1.44. Wang et al., 2023

In this study, Wang et al. (2023) performed cell level testing of LFP Li-ion batteries to gather data to be used in modeling of particle venting during thermal runaway. The cell used in the test was a 27 Ah/86.4 Wh, prismatic cell with a nominal voltage of 3.2 V. The mass of the cell was 625 g, and it was tested at 100% SOC.

The test utilized to quantify ejected particles was conducted in a sealed chamber and a heater was used to initiate thermal runaway. After completion of thermal runaway and venting of the cell, particles deposited on the chamber walls, battery, and heater surface were collected and sorted into particle size groups using mesh sieves. Based on information provided by the authors, it appears that flaming conditions were not achieved during the test. Of the total PM collected, 55% were 0 to 300 μm , 26% were 300 to 900 μm , 52% were 900 to 2000 μm , and 12% were greater than 2000 μm . The total settleable PM was 42.6 g and accounted for 6.8% of the starting cell mass. PM900 had a yield of 55 mg/g of the starting cell mass. Using a particle size analyzer, the authors determined that approximately 90% of raw, non-agglomerated particles were 349 μm or smaller, 50% were 141 μm or smaller, and 10% were 13 μm or smaller [85].

7.1.45. Willstrand et al., 2020

Research Institutes of Sweden (RISE) performed a study of combustion characteristics and toxic gases produced during combustion of BEVs and ICEVs. The analysis was divided into three parts- a literature review assessing both ICEVs and BEVs fires, full-scale fire testing on EVs, ICEVs, and Li-ion batteries, and FDS simulations of BEV fires in an underground parking garage. RISE was particularly interested in the production of HF gas during combustion of BEVs. The HF production was attributed to fluorinated materials in the vehicle battery packs, such as electrolytes containing LiPF_4 .

As part of the literature review, available data on full-scale vehicle fire testing peak HRR, THR, heat of combustion, and emissions was gathered. In addition, the peak HRR and THR from flaming thermal runaway of Li-ion batteries was obtained from previous fire testing of cells, cell arrays, and modules. Based on this analysis, it was concluded that there are no simple rules for estimating heat release rate of flaming thermal runaway of Li-ion batteries, especially for large batteries or battery packs. HRR depended on the type of battery, SOC, configuration of the cells, and how the cells are exposed. The data retrieved from the literature review for peak HRRs was plotted by Willstrand et al. (2020). The trend was not closely linear when considering the data sets independently. The same methodology was applied for total heat released and the correlation was found to be approximately linear, especially for assemblies with a high energy content.

A review of the BEV fire emissions found that HF was of particular concern. Other compounds identified PAH, polychlorinated dibenzo-p-dioxins (PCDD), heavy metals including nickel, manganese, cobalt, and lithium, asphyxiant gases such as CO and HCN, and irritant gases including HCl, SO_2 , and NO_2 being possible heat concerns.

Full-scale vehicle fire tests were performed on three vehicles below a collector hood: two EVs, referred to as BEV A and BEV B, and one ICEV, referred to as ICEV A. ICEV A (diesel engine)

and BEV A (pouch, NMC cells) were full-size vans of the same model and manufacturer. BEV-B (prismatic, NMC cells) was a small, family car from Manufacturer B. In the tests, both BEVs were at 80% SOC, and the ICEV contained 44 liters of fuel. The fuel for the ICEV was split between its fuel tank and a diesel pool located directly below the tank. The pool was ignited to simulate a realistic fire scenario. The BEVs were ignited via a 30-kW propane burner located under the battery pack. The burner remained active for the entire test duration. Gas yields were collected through the hood with a 24 m³/s flow rate. Gases including HF, HCl, HBr, CO₂, CO, HCN, SO₂, NO₂, and NO were analyzed via FTIR. Total hydrocarbons were analyzed via FID, and PAH were analyzed via XAD-2 sorbent tubes.

Gas yields measured in the exhaust duct were not significantly different between the three vehicles, except for the production of HF. It was observed that the yields of HF from the two BEVs (2.3 and 2.1 mg/g) were orders of magnitude higher than the yield from the ICEV (0.04 mg/g). HCN was detected in the tests for each of the three vehicles; however, the peak yield only exceeded the defined detection limit in the test for BEV B.

The authors reported the THR, mass loss, and effective heat of combustion for the ICEV and BEV tests. Contributions from the propane burner were excluded. ICEV A and BEV B have higher THR's compared to BEV A due to the larger combustible load in the full-sized vans. Mass loss was higher in BEV B due to the additional weight of the battery.

To evaluate scalability of testing, RISE performed small and medium scale fire tests of Li-ion batteries. These tests were performed using 40 Ah, prismatic, LMO/NMC cells with a capacity of 150 Wh and a nominal voltage of 3.9 V. The tests were performed in configurations of a single cell, two cells (300 Wh), a module (1.2 kWh), and a pack (8.4 kWh). The battery was at approximately 80% SOC. Emissions were sampled through a hood with a flow rate of 0.3, 1.0, and 12 m³/s for single cell, double cell and module, and battery pack, respectively. FTIR, NDIR, gas washing bottles with high-pressure ion chromatography (HPIC), and a paramagnetic analyzer were used to analyze gas emissions.

The results showed that total heat released had a linear relationship with electrical energy. However, the peak HRR of the tests was not linearly correlated to energy, because a larger amount of heat was released over a longer period. This was attributed to the typical characteristics of thermal runaway in which the battery cells are not induced into thermal runaway or vented at the same time. When merged with THR and peak HRR data from the literature review and full-scale vehicle tests, the data showed good agreement with the previous data. Additionally, the full-scale fire test and battery test data were relatively close to the line of best fit (48.5 kJ/Wh).

The gas production from the battery tests were measured via FTIR and gas-washing bottles. HF was detected in all tests. HCl and HBr were detected in the module and pack tests, and SO₂ and NO were detected in the module tests. The authors reported the quantities of gases detected in each test by FTIR. Plotting of the HF quantities measured in all the battery tests showed a linear trend between total HF produced and the energy of the batteries. The quantity of HF production attributed to the battery pack in the full vehicle tests was compared to the trendline established by the battery-only tests; the total amount of HF produced by the vehicle batteries, when mounted in a fully equipped vehicle, is less than what is expected. The observed HF production was close to the lower limit determined from the cell tests. The study pointed out that this may have been the result of wall losses, as HF typically reacts when it contacts materials. With the battery located in the vehicle, many material surfaces are present compared to the open air burning of the battery

cells and packs. Therefore, the probability of HF contacting a surface and reacting, prior to being transported in the plume, was greater [77].

7.1.46. Willstrand et al., 2023

Willstrand et al. (2023) performed tests on large format, prismatic NMC cells with a capacity of 157 Ah to determine whether SOC and the method of triggering thermal runaway affect gas production, mass loss, and thermal runaway onset. The cells were tested at 25, 50, 75, and 100% SOC, as well as an overcharge condition. The trigger methods were a heating ramp of 1 and 20°C/min, an external fire using a propane burner, a local heater, nail penetration, or overcharging. The fire tests were performed in both an inert, closed pressure vessel and a calorimeter open to ambient. In some tests, cells exploded, in which case, the results were excluded.

The cell SOC impacted total gas volume, gas production rate and composition, mass loss, thermal runaway onset and maximum temperatures. Thermal runaway onset temperatures tended to decrease by 18°C per 25% SOC, while maximum temperatures increased by 90°C per 25% SOC. As SOC increased, the percentage of mass loss also increased. However, mass loss due to vaporization and gas production was approximately 23% for all SOC. The thermal runaway trigger methods did not increase total gas production; however, more CO and less CO₂ was produced as SOC increased. HF was only detected in the open atmosphere, flaming experiments and the peak HF concentration detected in any test was 4.2 mg/Wh. SO₂, NO, NO₂, HCl, and HCN were analyzed for using FTIR but were not detected or were not quantifiable in any of the tests. A higher SOC was correlated with increased total gas volume and gas production per Ah.

The characteristic, or peak, gas production rate was found to be an average of approximately 130, 79, 73, 12, and 5 L/s for cells at overcharge, 100, 75, 50, and 25% SOC, respectively. Willstrand et al. (2023) concluded that trigger method and SOC both affected gas production rate, mass loss, and maximum temperature of the cell. The trigger method affected gas production rate, mass loss percentage, and maximum temperature. However, it did not seem to affect total gas volume produced or gas composition. Similar to the findings of others, Willstrand et al. (2023) indicated that the large cell format may enhance the effect of the trigger method and specific total gas production. Additionally, the authors found that surrounding pressure and temperature had a low impact on the characterization of thermal runaway [67].

7.1.47. Yang et al., 2022

In this study, gas production of Li-ion cells during thermal runaway was evaluated in an inert environment. The cells utilized in the tests included NMC cells with capacities of 50 Ah/215 Wh, 115 Ah/495 Wh, and 165 Ah/710 Wh and a total mass of 908, 1815, and 2158 g, respectively. Tests also included LFP cells with a capacity of 196 Ah/715 Wh and a total mass of 3349 g. All tests were of single cells at 100% SOC. The form of the cells (pouch, cylindrical, prismatic) was not identified in the publication. Thermal runaway was initiated via heating plates. The cells were tested in a sealed pressure chamber purged with nitrogen. Pressure and temperature measurements from within the chamber were used to calculate the volume of gases produced during thermal runaway, according to the ideal gas law. After thermal runaway, and after temperature and pressure reached a steady state, gases from within the chamber were sampled and analyzed with gas chromatography. Thermal runaway critical temperature was defined as the surface temperature of the cell at which the temperature rises sharply, and the cell enters thermal runaway. The cell gas

exhaust time was defined as the time from the opening of the cell valve to the end of the pressure relief of the cell.

The authors noted that the LFP cells had the lowest mass loss percentage and contributed this to the observation that the LFP cells ejected unreacted electrolytes while the NMC cells ejected black solid particles. The large mass loss percentage of the 165 Ah NMC cells was attributed to the ejection of internal coil materials during thermal runaway. HF was not detected in any of tests. The authors contributed this to the inert environment, which has a low water content, which did not allow PF_5 to react and be converted to HF. For CO , it was observed that concentrations increased linearly with capacity [60].

7.1.48. Yuan et al., 2020

NIOSH conducted 18 tests on cylindrical Li-ion cells with various chemistries to identify gases and concentrations released during thermal runaway. The cells utilized in the testing were LFP cells with a 3.8 Ah/12.2 Wh capacity and a mass of 90.1 g, LTO cells with a 1.3 Ah/3.1 Wh capacity and a mass of 38.6 g, and two types of NMC cells from different manufactures, both with a 3.2 Ah/11.7 Wh capacity and a nominal mass of 45 g. The cells tested via ARC. Thermal runaway was initiated via an electric heater applied to the canister containing the cell. Temperature and pressure within the canister were measured and used to calculate the total quantity of gas produced at ambient temperature and pressure. Gas samples were collected after thermal runaway and analyzed with gas chromatography. The gas analysis was not capable of detecting trace gases. The authors reported total gas production and percent volume of CO and CO_2 .

In identical tests conducted outside the canister, flaming was observed for the NMC cells but not for the LFP cells. Additional tests were also conducted for LFP single, 2-, and 3-cell bundles in a larger canister. The authors noted that the quantity of gas produced was very similar for the tests of single LFP cells in different size canisters (3.29 L and 3.79 L) and that the total gas quantity scaled proportionally with the number of cells tested. In the single cell test, in the smaller canister, the total volume of gas was released in approximately 15 seconds [61].

7.1.49. Zhang et al., 2019a

Zhang et al. (2019a) forced a 50 Ah, 3.65V, prismatic, NMC Li-ion cell at 100% SOC into thermal runaway via an external heater to characterize the settleable particulate matter released from the Li-ion battery. The mass of the cell was 870 g. The anode material was mainly graphite. The cathode current collector was aluminum foil, and the anode current collector was copper foil. The shell material of the cell was an aluminum alloy.

The test was conducted within a chamber purged with nitrogen. An element analyzer was used to detect carbon and sulfur, while fluorine was detected by a tester with a detection limit of 1 mg/kg. ICP-MS was used to detect nonradioactive metals, phosphorus, boron, and silicon with a detection limit of 1 mg/kg. Thermal runaway was found to initiate at 167°C and the temperatures measured in the vent gas jet zone were found to reach a peak of 350°C. Vent gases were sampled at 185°C (VG185) and then reheated for detection at 90°C (VG90). The VG90 was analyzed using gas chromatography for CO , CO_2 , H_2 , and hydrocarbons. GC-MS was used to detect DMC, DEC, and EMC. Ion chromatography was used for HCl .

Vent gases were categorized by the temperature at which they were stable. Seventeen gases were stable at 25°C (VG25), eight were stable from 25°C to 90°C (VG25 to VG90), and six gases were stable from 90°C to 185°C (VG90 to VG185). The vent gases have a wide distribution of boiling points. The majority of VG90 emissions were made of CO, CO₂, and H₂. Hydrocarbons were present, but at a much smaller percentage. The total amount of vent gas was determined to be 3.83 mol. A total of 876, 1031, 2.02, and less than 0.13 mmol of CO₂, CO, Benzene, and HCl were produced, respectively.

Overall, the total mass lost was 248.2 g, approximately 28.53% of the total cell mass. Settleable PM made up 17% of the total emissions. VG25 made up 32.52% and VG90 to VG185 plus dust made up 50.25% of the total emissions. The rest was composed of VG25 to VG90 (0.23%) [81].

7.1.50. Zhang et al., 2019b

Zhang et al. (2019b) conducted a complimentary analysis to Zhang et al. (2019a) using the same experimental setup except for the total cell mass which was 900 g. Cells were forced into thermal runaway via an external heater to characterize the gaseous and solid composition of effluents released from a Li-ion battery during non-flaming thermal runaway. The shell material of the cell was an aluminum alloy. As a follow-up to this experiment and Zhang et al. (Nov. 2019a), testing was performed by Wang et al. (2020).

The test was conducted within a chamber purged with nitrogen and all PM that settled within the chamber was collected after termination of the thermal runaway event. The PM was analyzed using a million point electronic balance and sample sieves to determine mass distribution. A particle size analyzer was used. An element analyzer was used to detect carbon and sulfur, while fluorine was detected by a tester with a detection limit of 1 mg/kg. ICP-MS was used to detect nonradioactive metals, phosphorus, boron, and silicon with a detection limit of 1 mg/kg.

The total mass of settleable PM was 97.47 g (11.20% cell mass). Of the PM collected, 43.79% were 0.0029 to 0.85 mm, 36.37% were 0.85 to 1.70 mm, 8.88% were 1.70 to 2.00 mm, and 10.96% were 2.00 to 8.50 mm by mass. the majority of settleable PM (90%) was larger than 22.55 μm. PM850 had a yield of 47 mg/g of the starting cell mass. Metallic elements made up 42.9% of the total settleable PM mass. Nickel, copper, cobalt, manganese, aluminum, and lithium accounted for 30.21%, 17.19%, 7.08%, 5.59%, 4.94%, 4.00%, and 3.05% of the total settleable PM mass, respectively. In the smaller PM diameter range (0 to 850 μm), carbon (30.08%) and nickel (18.13%) made up most of the sample, followed by cobalt (5.91%), copper (5.75%), manganese (5.25%), aluminum (3.63%), and lithium (2.90%). The authors concluded that the settleable PM contained elements potentially toxic to humans [86].

7.1.51. Zhang et al., 2022

In an evaluation of the effect of water spray on combustion of Li-ion cells, Zhang et al. (2022) performed thermal runaway tests on NMC cells, during which some had no water spray applied. The cells utilized in the test were cylindrical cells with a capacity of 4 Ah/14.8 Wh and a mass of 68.5 g.

Cells were tested at 0, 50, and 100% SOC in the experiments without an applied water spray. The tests conducted with a water spray all utilized cells at 100%SOC. Thermal runaway was initiated via a cylindrical heater adjacent to the cell. Tests were conducted in an explosion proof

tank within a combustion chamber equipped with a collection hood and exhaust system. Gas was sampled from the exhaust duct for the duration of the tests and analyzed via FTIR.

The cell at 0% SOC did not achieve thermal runaway but did vent limited amounts of gas. The cells at 50 and 100% SOC underwent flaming thermal runaway. In the 100% SOC test, the cell experienced a violent ejection of material particles, followed by a jet fire. The ejection of solid materials explained the increased mass loss percentage of 41.5% versus 10.8% and 19.4% in the 0 and 50% SOC tests. The authors reported the thermal runaway onset temperature, mass loss, species total gas production and gas production rate at various SOC. The authors noted that total CO production increased with increasing SOC while total CO₂ production, and this was attributed to more incomplete combustion in the higher SOC tests. Zhang et al. (2022) concluded that the toxicity of the generated gases increased with the application of water spray, particularly due to increased production of HF [79].

7.2. Emissions Tables

Table 37. LFP non-flaming yields.

Source	% Volume										Mass Produced [mg/wh]										Gas Measurement Methods
	HF	CO	CO ₂	HBr	HCl	NO ₂	SO ₂	HCN	NH ₃	Ben	HF	CO	CO ₂	HBr	HCl	NO ₂	SO ₂	HCN	NH ₃	Ben.	
Archibald (2021) [56]	-	7.8	24.0	-	-	-	-	-	-	-	-	35.3	73.9	-	-	-	-	-	-	-	GC-TCD
Gully (2019) [57]	1.6	7.6	44.3	-	1.1	4.9	-	0.1	-	0.0	16.4	108.7	995.9	-	-	115.1	-	1.4	-	0.0	FTIR
Gully (2019) [57]	1.6	15.9	20.2	-	0.8	9.7	-	0.1	-	0.7	11.4	159.3	317.9	-	-	159.6	-	1.0	-	19.6	FTIR
Gully (2019) [57]	0.1	26.1	20.9	-	0.3	1.3	-	0.1	-	13.6	2.1	784.2	986.7	-	-	64.1	-	2.9	-	1139.6	FTIR
Gully (2019) [57]	1.9	12.0	22.5	-	2.1	4.8	-	0.4	-	0.6	16.2	143.1	421.5	-	-	94.0	-	4.6	-	20.0	FTIR
Gully (2019) [57]	3.7	13.9	23.0	-	1.9	5.6	-	0.7	-	0.0	31.5	165.7	430.9	-	-	109.7	-	8.1	-	0.0	FTIR
Golubkov (2014) [58]	-	4.8	53.0	-	-	-	-	-	-	-	-	19.2	30.2	-	-	-	-	-	-	-	GC
Golubkov (2015) [59]	-	1.8	93.5	-	-	-	-	-	-	-	-	7.9	642.8	-	-	0.0	-	-	-	-	GC
Golubkov (2015) [59]	-	3.1	85.3	-	-	-	-	-	-	-	-	7.6	330.5	-	-	-	-	-	-	-	GC
Golubkov (2015) [59]	-	4.8	66.2	-	-	-	-	-	-	-	-	12.2	264.8	-	-	-	-	-	-	-	GC
Golubkov (2015) [59]	-	6.4	62.6	-	-	-	-	-	-	-	-	20.9	320.8	-	-	-	-	-	-	-	GC
Golubkov (2015) [59]	-	9.1	48.3	-	-	-	-	-	-	-	-	23.2	193.2	-	-	-	-	-	-	-	GC
Golubkov (2015) [59]	-	6.4	52.2	-	-	-	-	-	-	-	-	28.1	398.0	-	-	-	-	-	-	-	GC
Golubkov (2015) [59]	-	7.7	55.8	-	-	-	-	-	-	-	-	35.5	404.6	-	-	-	-	-	-	-	GC
Huang (2021) [55]	-	-	-	-	-	-	-	-	-	-	0.0	6.4	13.5	-	4.0	-	-	-	3.9	-	FTIR, HF Detector
Sturk (2019) [8]	-	-	-	-	-	-	-	-	-	-	26.0 ¹	-	-	-	-	-	-	-	-	-	FTIR, Wash Bottles
Yang (2022) [60]	0.0	10.0	26.0	-	-	-	-	-	-	-	0.0	38.4	168.9	-	-	-	-	-	-	-	GC
Yuan (2020) [61]	-	4.5	25.4	-	-	-	-	-	-	-	-	15.2	134.5	-	-	-	-	-	-	-	GC
Proprietary Data ²	-	11.0	29.0	-	-	-	-	-	-	0.004	-	-	-	-	-	-	-	-	-	-	GC

Ben: Benzene

¹Average of results produced by FTIR and wash bottle methods

²Data sourced from a proprietary testing report of a module used in a commercial BESS

Table 38. NMC non-flaming yields.

Source	% Volume										Mass Produced [mg/wh]										Gas Measurement Methods
	HF	CO	CO ₂	HBr	HCl	NO ₂	SO ₂	HCN	NH ₃	Ben	HF	CO	CO ₂	HBr	HCl	NO ₂	SO ₂	HCN	NH ₃	Ben.	
Amano (2023) [62]	-	-	-	-	-	-	-	-	-	-	0.001	1.2	0.0	-	-	-	-	0.005	-	-	FTIR
Amano (2023) [62]	-	-	-	-	-	-	-	-	-	-	0.002	3.4	0.0	-	-	-	-	0.01	-	-	FTIR
Amano (2023) [62]	-	-	-	-	-	-	-	-	-	-	0.004	5.0	6.4	-	-	-	-	0.03	-	-	FTIR
Archibald (2021) [56]	-	21.3	29.9	-	-	-	-	-	-	-	-	170.6	376.2	-	-	-	-	-	-	-	GC-TCD
Bordes (2022) [63]	-	-	-	-	-	-	-	-	-	-	1.0	77.1	358.6	-	-	-	-	-	-	-	NDIR, CLD, FTIR
Gully (2019) [57]	0.7	29.2	19.6	-	9.7	-	-	0.0	-	4.1	11.6	675.0	711.9	-	-	-	-	0.0	-	264.3	FTIR
Gully (2019) [57]	0.1	19.0	65.9	-	0.2	-	-	0.0	-	1.9	0.8	213.8	1165	-	-	-	-	0.0	-	59.6	FTIR
Essl (2020a) [64]	0.0	17.0	38.0	-	-	-	-	-	-	-	0.0	77.6	273.1	-	-	-	-	-	-	-	FTIR, GC
Essl (2020b) [65]	0.0	26.0	30.0	-	-	-	-	-	-	-	0.0	141.2	256.5	-	-	-	-	-	-	-	FTIR, GC
Essl (2020b) [65]	0.0	33.0	20.0	-	-	-	-	-	-	-	0.0	319.0	303.7	-	-	-	-	-	-	-	FTIR, GC
Essl (2020b) [65]	0.0	22.0	30.0	-	-	-	-	-	-	-	0.0	131.0	281.0	-	-	-	-	-	-	-	FTIR, GC
Essl (2020b) [65]	0.0	30.0	21.0	-	-	-	-	-	-	-	0.0	163.0	179.6	-	-	-	-	-	-	-	FTIR, GC
Essl (2020b) [65]	0.0	30.0	20.0	-	-	-	-	-	-	-	0.0	275.9	288.9	-	-	-	-	-	-	-	FTIR, GC
Essl (2020b) [65]	0.0	23.0	24.0	-	-	-	-	-	-	-	0.0	141.2	231.5	-	-	-	-	-	-	-	FTIR, GC
Golubkov (2014) [58]	-	27.6	24.9	-	-	-	-	-	-	-	-	206.9	293.3	-	-	-	-	-	-	-	GC
Golubkov (2014) [58]	-	13.0	41.2	-	-	-	-	-	-	-	-	95.2	474.0	-	-	-	-	-	-	-	GC
Huang (2020) [54]	-	-	-	-	-	-	-	-	-	-	-	19.1	149.4	-	-	-	30.8	-	1.7	-	FTIR

Sturk (2019) [8]	-	-	-	-	-	-	-	-	-	-	14.3 ¹	-	-	-	-	-	-	-	-	-	FTIR, Wash Bottles
Willstrand (2023) [67]	0.0	-	-	-	0.0	0.0	0.0	0.0	-	-	-	-	-	-	-	-	-	-	-	-	FTIR
Willstrand (2023) [67]	0.0	44.0	22.0	-	0.0	0.0	0.0	0.0	-	-	-	-	-	-	-	-	-	-	-	-	FTIR
Willstrand (2023) [67]	0.0	36.0	28.0	-	0.0	0.0	0.0	0.0	-	-	-	-	-	-	-	-	-	-	-	-	FTIR
Willstrand (2023) [67]	0.0	26.0	48.0	-	0.0	0.0	0.0	0.0	-	-	-	-	-	-	-	-	-	-	-	-	FTIR
Willstrand (2023) [67]	0.0	13.0	58.0	-	0.0	0.0	0.0	0.0	-	-	-	-	-	-	-	-	-	-	-	-	FTIR
Yang (2022) [60]	0.0	32.4	35.3	-	-	-	-	-	-	-	0.0	149.8	204.7	-	-	-	-	-	-	-	GC
Yang (2022) [60]	0.0	29.6	28.1	-	-	-	-	-	-	-	0.0	201.7	296.5	-	-	-	-	-	-	-	GC
Yang (2022) [60]	0.0	60.3	13.0	-	-	-	-	-	-	-	0.0	410.1	143.2	-	-	-	-	-	-	-	GC
Zhang (2019a) [81]	-	-	-	-	-	-	-	-	-	-	-	158.2	211.2	-	0.02	-	-	-	-	0.9	GC, IC

Ben: Benzene

¹Average of results produced by FTIR and wash bottle methods

Table 39. LFP flaming yields.

Source	Mass Produced [mg/g]										Mass Produced [mg/Wh]										Gas Measurement Methods
	HF	CO	CO ₂	HBr	HCl	NO ₂	SO ₂	HCN	NH ₃	Ben.	HF	CO	CO ₂	HBr	HCl	NO ₂	SO ₂	HCN	NH ₃	Ben.	
Andersson (2013) [18]	14.2	-	-	-	-	-	-	-	-	-	43.8	-	-	-	-	-	-	-	-	-	FTIR
Andersson (2013) [18]	18.4	-	-	-	-	-	-	-	-	-	56.3	-	-	-	-	-	-	-	-	-	FTIR
Andersson (2013) [18]	16.7	-	-	-	-	-	-	-	-	-	50.9	-	-	-	-	-	-	-	-	-	FTIR
Andersson (2013) [18]	32.0	-	-	-	-	-	-	-	-	-	100.9	-	-	-	-	-	-	-	-	-	FTIR
Andersson (2013) [18]	39.3	-	-	-	-	-	-	-	-	-	124.1	-	-	-	-	-	-	-	-	-	FTIR
Andersson (2013) [18]	15.2	-	-	-	-	-	-	-	-	-	23.9	-	-	-	-	-	-	-	-	-	FTIR
Gully (2019) [57]	-	-	-	-	-	-	-	-	-	-	9.4	499.1	3293	-	-	320.3	-	0.0	-	0.0	FTIR
Gully (2019) [57]	-	-	-	-	-	-	-	-	-	-	36.8	161.7	789.1	-	-	115.1	-	8.3	-	12.0	FTIR
Larsson (2016) [68]	15.2	-	-	-	-	-	-	-	-	-	23.9	-	-	-	-	-	-	-	-	-	FTIR
Larsson (2016) [68]	7.1	-	-	-	-	-	-	-	-	-	12.0	-	-	-	-	-	-	-	-	-	FTIR
Larsson (2016) [68]	18.7	-	-	-	-	-	-	-	-	-	57.6	-	-	-	-	-	-	-	-	-	FTIR
Larsson (2017) [69]	-	-	-	-	-	-	-	-	-	-	166.8 ¹	-	-	-	-	-	-	-	-	-	FTIR, Wash Bottles
Larsson (2017) [69]	-	-	-	-	-	-	-	-	-	-	53.9	-	-	-	-	-	-	-	-	-	FTIR
Larsson (2017) [69]	-	-	-	-	-	-	-	-	-	-	141.3	-	-	-	-	-	-	-	-	-	FTIR
Larsson (2017) [69]	-	-	-	-	-	-	-	-	-	-	23.9	-	-	-	-	-	-	-	-	-	FTIR
Larsson (2017) [69]	-	-	-	-	-	-	-	-	-	-	52.3	-	-	-	-	-	-	-	-	-	FTIR
Lecocq (2016) [129]	-	-	-	-	-	-	-	-	-	-	49.3	87.1	-	-	-	-	0.0	-	-	-	FTIR

Lecocq (2016) [129]	-	-	-	-	-	-	-	-	-	-	84.8	71.0	-	-	-	-	0.0	-	-	-	FTIR
Lecocq (2016) [129]	-	-	-	-	-	-	-	-	-	-	104.0	56.0	-	-	-	-	0.0	-	-	-	FTIR
Lecocq (2016) [129]	-	-	-	-	-	-	-	-	-	-	2.4	66.4	-	-	-	-	28.1	-	-	-	FTIR
Lecocq (2016) [129]	-	-	-	-	-	-	-	-	-	-	3.3	46.9	-	-	-	-	33.8	-	-	-	FTIR
Lecocq (2016) [129]	-	-	-	-	-	-	-	-	-	-	11.2	26.0	-	-	-	-	47.6	-	-	-	FTIR
Liu (2020) [70]	2.9	30.2	1518	-	-	-	-	-	-	-	4.1	42.3	2126	-	-	-	-	-	-	-	Gas Analyzer, Optical Sensor
Liu (2020) [70]	6.8	31.9	1170	-	-	-	-	-	-	-	10.8	50.7	1858	-	-	-	-	-	-	-	Gas Analyzer, Optical Sensor
Liu (2020) [70]	19.2	41.5	41.5	-	-	-	-	-	-	-	37.1	80.0	80.0	-	-	-	-	-	-	-	Gas Analyzer, Optical Sensor
Liu (2021) [71]	1.7	3.6	731.9	-	0.8	0.4	1.9	-	0.5	-	2.1	4.4	884.3	-	0.9	0.4	2.2	-	0.6	-	Gas Analyzer, FTIR
Liu (2021) [71]	2.8	6.0	784.0	-	0.7	0.5	2.3	-	0.5	-	3.6	7.6	993.6	-	0.9	0.6	2.9	-	0.6	-	Gas Analyzer, FTIR
Liu (2021) [71]	7.1	10.8	1482	-	0.7	2.3	3.8	-	0.5	-	10.4	15.8	2163	-	1.0	3.4	5.6	-	0.7	-	Gas Analyzer, FTIR
Meng (2020) [72]	-	-	-	-	-	-	-	-	-	-	4.9	56.8	1931	-	-	-	-	-	-	-	Gas Analyzer, Optical Sensor
Meng (2020) [72]	-	-	-	-	-	-	-	-	-	-	17.3	104.9	1821	-	-	-	-	-	-	-	Gas Analyzer, Optical Sensor
Meng (2020) [72]	-	-	-	-	-	-	-	-	-	-	28.4	34.6	1559	-	-	-	-	-	-	-	Gas Analyzer, Optical Sensor
Sturk (2015) [74]	-	-	-	-	-	-	-	-	-	-	67.0 ²	-	-	-	-	-	-	-	-	-	FTIR, Wash Bottles
Sturk (2015) [74]	-	-	-	-	-	-	-	-	-	-	40.2 ²	-	-	-	-	-	-	-	-	-	FTIR, Wash Bottles
Sturk (2015) [74]	-	-	-	-	-	-	-	-	-	-	110.7 ²	-	-	-	-	-	-	-	-	-	FTIR, Wash Bottles
Sturk (2015) [74]	-	-	-	-	-	-	-	-	-	-	50.0 ²	-	-	-	-	-	-	-	-	-	FTIR, Wash Bottles

Sturk (2015) [74]	-	-	-	-	-	-	-	-	-	-	104.5 ²	-	-	-	-	-	-	-	-	-	FTIR, Wash Bottles
Sturk (2015) [74]	-	-	-	-	-	-	-	-	-	-	107.1 ²	-	-	-	-	-	-	-	-	-	FTIR, Wash Bottles
Sturk (2015) [74]	-	-	-	-	-	-	-	-	-	-	127.7 ²	-	-	-	-	-	-	-	-	-	FTIR, Wash Bottles
Sturk (2015) [74]	-	-	-	-	-	-	-	-	-	-	167.9 ²	-	-	-	-	-	-	-	-	-	FTIR, Wash Bottles
Sturk (2015) [74]	-	-	-	-	-	-	-	-	-	-	183.5 ²	-	-	-	-	-	-	-	-	-	FTIR, Wash Bottles

Ben: Benzene

¹Average of results produced by FTIR and wash bottle methods

²Results are reported as total quantities detected by both FTIR and gas wash bottles simultaneously

Table 40. NMC flaming yields.

Source	Mass Produced [mg/g]										Mass Produced [mg/Wh]										Gas Measurement Methods
	HF	CO	CO ₂	HBr	HCl	NO ₂	SO ₂	HCN	NH ₃	Ben.	HF	CO	CO ₂	HBr	HCl	NO ₂	SO ₂	HCN	NH ₃	Ben.	
Amano (2023) [62]	-	-	-	-	-	-	-	-	-	-	0.01	45.7	365.0	-	-	-	-	0.1	-	-	FTIR
Amano (2023) [62]	-	-	-	-	-	-	-	-	-	-	0.01	59.5	663.5	-	-	-	-	0.1	-	-	FTIR
Amano (2023) [62]	-	-	-	-	-	-	-	-	-	-	-	17.3	-	-	-	-	-	0.1	-	-	FTIR
Amano (2023) [62]	-	-	-	-	-	-	-	-	-	-	-	16.3	-	-	-	-	-	0.1	-	-	FTIR
Amano (2023) [62]	-	-	-	-	-	-	-	-	-	-	-	59.2	22.3	-	-	-	-	0.3	-	-	FTIR
Amano (2023) [62]	-	-	-	-	-	-	-	-	-	-	-	49.0	-	-	-	-	-	0.1	-	-	FTIR
Amano (2023) [62]	-	-	-	-	-	-	-	-	-	-	-	49.8	-	-	-	-	-	0.1	-	-	FTIR
Amano (2023) [62]	-	-	-	-	-	-	-	-	-	-	-	205.0	-	-	-	-	-	0.1	-	-	FTIR
Amano (2023) [62]	-	-	-	-	-	-	-	-	-	-	-	147.8	-	-	-	-	-	0.3	-	-	FTIR
Amano (2023) [62]	-	-	-	-	-	-	-	-	-	-	-	134.7	-	-	-	-	-	0.2	-	-	FTIR
Amano (2023) [62]	-	-	-	-	-	-	-	-	-	-	-	160.7	-	-	-	-	-	0.4	-	-	FTIR
Blum & Long (2016) [125]	-	-	-	-	-	-	-	-	-	-	0.02	-	-	-	-	-	-	-	-	-	Portable Detector
Bordes (2022) [63]	-	-	-	-	-	-	-	-	-	-	6.7	109.5	2797	-	-	5.7	-	-	-	-	NDIR, CLD, FTIR
Bordes (2022) [63]	-	-	-	-	-	-	-	-	-	-	16.2	67.6	-	-	-	2.4	-	-	-	-	NDIR, CLD, FTIR
Gully (2019) [57]	-	-	-	-	-	-	-	-	-	-	2.1	111.0	616.8	-	-	-	-	0.0	-	29.9	FTIR
Gully (2019) [57]	-	-	-	-	-	-	-	-	-	-	0.7	345.5	612.3	-	-	-	-	0.0	-	120.4	FTIR
Gully (2019) [57]	-	-	-	-	-	-	-	-	-	-	2.1	371.1	393.3	-	-	-	-	0.0	-	141.3	FTIR
Forestier (2020) [127]	-	-	-	-	-	-	-	-	-	-	9.3	111.1	463.0	-	-	-	-	-	-	-	FTIR

Huang (2020) [54]	-	-	-	-	-	-	-	-	-	-	-	133.3	341.3	-	-	-	15.2	-	0.9	-	FTIR
Huang (2021) [55]	0.8	19.7	423.3	-	0.4	-	-	-	0.0	-	2.0	47.5	1023	-	0.9	-	-	-	0.0	-	FTIR, HF Detector
Sturk (2015) [74]	-	-	-	-	-	-	-	-	-	-	14.5 ¹	-	-	-	-	-	-	-	-	-	FTIR, Wash Bottles
Sturk (2015) [74]	-	-	-	-	-	-	-	-	-	-	6.2 ¹	-	-	-	-	-	-	-	-	-	FTIR, Wash Bottles
Sturk (2015) [74]	-	-	-	-	-	-	-	-	-	-	11.3 ¹	-	-	-	-	-	-	-	-	-	FTIR, Wash Bottles
Sturk (2015) [74]	-	-	-	-	-	-	-	-	-	-	8.7 ¹	-	-	-	-	-	-	-	-	-	FTIR, Wash Bottles
Sturk (2015) [74]	-	-	-	-	-	-	-	-	-	-	18.9 ¹	-	-	-	-	-	-	-	-	-	FTIR, Wash Bottles
Willstrand (2020) [77]	-	-	-	-	-	-	-	-	-	-	29.0	29.8	-	0.6	1.3	-	-	-	-	-	FTIR
Willstrand (2020) [77]	-	-	-	-	-	-	-	-	-	-	41.7	11.7	3917	0.1	1.6	1.8	15.0	-	-	-	FTIR
Willstrand (2020) [77]	-	-	-	-	-	-	-	-	-	-	35.0	6.0	-	-	1.7	0.9	18.3	-	-	-	FTIR
Willstrand (2020) [77]	-	-	-	-	-	-	-	-	-	-	36.7	1.0	3100	-	-	-	-	-	-	-	FTIR
Willstrand (2020) [77]	-	-	-	-	-	-	-	-	-	-	30.3	1.3	-	-	-	-	-	-	-	-	FTIR
Willstrand (2020) [77]	-	-	-	-	-	-	-	-	-	-	23.3	0.7	-	-	-	-	-	-	-	-	FTIR
Willstrand (2020) [77]	-	-	-	-	-	-	-	-	-	-	26.7	1.3	-	-	-	-	-	-	-	-	FTIR
Willstrand (2020) [77]	-	-	-	-	-	-	-	-	-	-	32.0	2.0	-	-	-	-	-	-	-	-	FTIR
Willstrand (2020) [77]	-	-	-	-	-	-	-	-	-	-	34.0	1.3	-	-	-	-	-	-	-	-	FTIR
Willstrand (2023) [67]	-	-	-	-	-	-	-	-	-	-	4.2	-	-	-	-	-	-	-	-	-	FTIR
Yuan (2020) [61]	-	-	-	-	-	-	-	-	-	-	-	316.4	216.9	-	-	-	-	-	-	-	GC
Yuan (2020) [61]	-	-	-	-	-	-	-	-	-	-	-	358.8	370.4	-	-	-	-	-	-	-	GC
Zhang (2022) [79]	7.5	30.1	315.8	-	-	-	-	-	-	-	6.8	27.0	283.8	-	-	-	-	-	-	-	FTIR

Zhang (2022) [79]	7.0	45.8	45.8	-	-	-	-	-	-	-	13.5	87.8	87.8	-	-	-	-	-	-	FTIR
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Ben: Benzene
¹Results are reported as total quantities detected by both FTIR and gas wash bottles simultaneously

Table 41. Particulate matter composition for various cell chemistries and thermal runaway conditions.

Li-Ion Battery Characteristics				Particulate Matter Composition (% mass)														Analysis Method	Source
Chem.	Geom.	Cap.	TR Conditions	Li	Ni	Co	Mn	Al	Cr	Cu	Zn	Fe	Zr	Sr	Na	Ca	Ti		
NMC ^a	Pouch	70 Wh	Non-Flaming	6	30	23	19	9	-	0	-	-	-	-	-	-	-	ICP-OES	Bordes et. al. (2022) [63]
NMC ^a	Pouch/Array (3 cells)	210 Wh	Flaming	5	27	20	19	6	-	0	-	-	-	-	-	-	-	ICP-OES	Bordes et. al. (2022) [63]
NMC ^a	Pouch/Module (9 cells)	210 Wh	Flaming	6	32	23	19	6	-	0	-	-	-	-	-	-	-	ICP-OES	Bordes et. al. (2022) [63]
NMC	Prismatic	90 Ah	Flaming	3-4	18-20	18-20	18-20	-	-	-	-	-	-	-	-	-	-	SEM-EDX, ED-XRF	Held et. al. (2022) [110]
NMC ^b	Prismatic	183 Wh	Non-Flaming	-	41.42	-	-	-	0.002	6.54	0.002	-	-	-	-	-	-	ICP-MS	Wang et. al. (2020) [84]
NMC ^c	Prismatic	183 Wh	Non-Flaming	2.90	18.13	5.91	5.25	3.63	0.07	5.75	0.007	0.51	0.01	0.03	0.07	0.04	0.01	ICP-MS	Zhang et. al. (2019a) [81]
NMC ^b	Prismatic	183 Wh	Non-Flaming	3.64	20.75	6.96	6.34	9.38	0.004	9.47	0.01	0.08	0.06	0.06	0.06	0.04	0.01	ICP-MS	Zhang et. al. (2019b) [86]

TR: thermal runaway

- a) Mass percentages for inorganic PM only (i.e. does not consider the presence of carbon)
- b) Mass percentages for PM ranging from 0 to 500 μm .
- c) Mass percentages for PM ranging from 0 to 850 μm .

7.3. IDLH Justifications

The following justification for the benzene IDLH value is an excerpt from the NIOSH IDLH [92].

“The chosen IDLH is based on the report in Patty [1963] that for man, a single exposure to 3,000 ppm is endurable for 0.5 to 1 hour [Flury 1928].”

The following justification for the CO IDLH value is an excerpt from the NIOSH IDLH [92].

“The chosen IDLH is based on the statement by Patty [1963] that a 1-hour exposure to 1,000 to 1,200 ppm would cause unpleasant, but no dangerous symptoms [Henderson et al. 1921]. Patty [1963] also reported that 1,500 to 2,000 ppm might be a dangerous concentration for an exposure of 1 hour [Henderson et al. 1921].”

The following justification for the CO₂ IDLH value is an excerpt from the NIOSH IDLH [92].

“The chosen IDLH is based on the statements by ACGIH [1971] that a 30-minute exposure at 50,000 ppm produces signs of intoxication, and a few minutes of exposure at 70,000 ppm and 100,000 ppm produces unconsciousness [Flury and Zernik 1931]. AIHA [1971] reported that 100,000 ppm is the atmospheric concentration immediately dangerous to life. In addition, Hunter [1975] noted that exposure to 100,000 ppm for only a few minutes can cause loss of consciousness.”

The following justification for the HBr IDLH value is an excerpt from the NIOSH IDLH [92].

“Hydrogen bromide is an extremely irritating and corrosive gas. The chosen IDLH is based on an analogy with bromine. According to ILO [1971], however, bromine produces a more marked toxic action. AIHA [1958] reported that for humans, 40 to 60 ppm bromine is dangerous for short exposure [Henderson and Haggard 1943]. Because hydrogen bromide is considered less irritating than bromine, an IDLH of 50 ppm is chosen.”

The following justification for the HCl IDLH value is an excerpt from the NIOSH IDLH [92].

“The chosen IDLH is based on the statements by Patty [1963] that according to Matt [1889] as cited in Flury and Zernik [1931], work is impossible when one inhales air containing hydrogen chloride in concentrations of 75 to 150 mg/m³ (50 to 100 ppm); work is difficult but possible when the air contains concentrations of 15 to 75 mg/m³ (10 to 50 ppm); and work is undisturbed at the concentration of 15 mg/m³ (10 ppm).”

The following justification for the HCN IDLH value is an excerpt from the NIOSH IDLH [92].

“The chosen IDLH is based on the statements by Patty [1963] that 45 to 54 ppm is ‘tolerated by man for 0.5 to 1 hour without immediate or late effects; 110 to 135 ppm, however, may be fatal after 0.5 to 1 hour or later, or dangerous to life [Flury and Zernik 1931; Dudley et al. 1942].”

The following justification for the HF IDLH value is an excerpt from the NIOSH IDLH [92].

“The chosen IDLH is based on the statement by Patty [1963] that 24 mg/m³ (30 ppm) was tolerated by animals for a total of 41 hours without a fatality [Machle et al. 1934]. A concentration of 50 ppm is obviously too high to be selected as the IDLH, because Deichmann and Gerarde [1969] stated that 50 ppm may be fatal when inhaled for 30 to 60 minutes.”

The following justification for the NH₃ IDLH value is an excerpt from the NIOSH IDLH [92].

“The chosen IDLH is based on the statement by AIHA [1971] that 300 to 500 ppm for 30 to 60 minutes have been reported as a maximum short exposure tolerance [Henderson and Haggard 1943]. AIHA [1971] also reported that 5,000 to 10,000 ppm are reported to be fatal [Mulder and Van der Zahm 1967] and exposures for 30 minutes to 2,500 to 6,000 ppm are considered dangerous to life [Smyth 1956].”

The following justification for the NO₂ IDLH value is an excerpt from NIOSH (2017) [132].

“Nitrogen dioxide is an irritant to the mucous membranes and has been shown to cause coughing and dyspnea during exposure. Severe exposure pulmonary edema with symptoms of chest pain, cough, dyspnea, and cyanosis have been reported [NIOSH 1976; Douglas et al. 1989]. Human data indicate that acute inhalation exposures may induce potential escape-impairing effects of dyspnea, cyanosis, and pulmonary edema [Henschler et al. 1960; Norwood et al. 1969; Morley and Silk 1970]. Exposure to nitrogen dioxide at 30 ppm for 70 minutes resulted in a severe cough and an increased burning sensation of the upper respiratory tract that progressed with continued exposures to include the lower section of the airways and in the chest [Henschler et al. 1960]. These effects can be considered a LOAEL and serve as the basis of the IDLH value for nitrogen dioxide. Duration adjustment (see Table 5) resulted in the calculation of a 30-minute equivalent concentration of 38 ppm. Application of a composite uncertainty factor of 3 to account for human variability yielding an IDLH value 13 ppm for nitrogen dioxide.”

The following justification for the SO₂ IDLH value is an excerpt from the NIOSH IDLH [92].

“The chosen IDLH is based on the statement by AIHA [1955] that 50 to 100 ppm is considered the maximum concentration for exposures of 0.5 to 1 hour [Henderson and Haggard 1943]. With regard to the atmospheric concentration immediately hazardous to life, AIHA [1955] reported that 400 to 500 ppm is considered dangerous for even short periods of exposure [Henderson and Haggard 1943] and that exposure to unendurable concentrations is not necessarily hazardous if escape is made within a few minutes.”

7.4. AEGL-1 Justifications

The following justification for the benzene AEGL-1 values is an excerpt from the Committee on Acute Exposure Guideline Levels (2009) [133].

“Although CNS effects of benzene are already known for over 100 years, very little is known about the time-concentration-effect relationship of slight CNS effects due to benzene exposure in humans, and no quantitative point of departure is available for a solid PBPK modeling. Although the study by Srbova et al. (1950) has some weaknesses (no details on all individual exposures and time durations, the lack of symptoms was reported by a single remark, no active investigation of health effects), the 110 ppm level for 2h is taken as a NOEL for CNS effects. This is the starting point for AEGL-1 development. This NOEL appears to be supported by the fact that a substantial number of volunteers was exposed in a controlled or occupational setting to levels of 1 – 76 ppm for 7h TWA (Inoue et al., 1986; 64 men, 88 women, occupational), 32 ppm ± 25 ppm for 8h TWA (Inoue et al., 1988; 65 workers, occupational) or 19-125 ppm for 6-8h (Hunter and Blair, 1972; male laboratory staff, controlled exp.) although none of these studies actually included statements on health effects. Because CNS effects are the consequence of systemic benzene exposure, time extrapolation should be applied. Based on the experiments described by Von Oettingen (1940) with cats, a n-value of 1 was identified for light and deep narcosis in cats (see section 6.2).

Although these data from cats are from an old experiment and details about the experiment are lacking, the extensive number of concentrations and time points reported provides sufficient confidence in the results indicating that using $N=3$ for extrapolation to short time periods is too conservative. Therefore, time extrapolation is performed using $N=1$ and $N=2$ for longer and shorter time periods respectively. Because human data are used, the interspecies uncertainty factor is 1. The intraspecies uncertainty factor is 3 because it has been found from experience with anesthetic gases that CNS depression does not vary by more than a factor 2-3 between groups in the population.”

The following justification for the HBr AEGL-1 values is an excerpt from the Committee on Acute Exposure Guideline Levels (2014) [134].

“The threshold for nasal irritation of 3ppm in human subjects exposed to HBr for several minutes (CT Department of Health, unpublished data, 1955, as cited in ACGIH 2002) was selected as the basis for the AEGL-1 values. That concentration was considered to be a threshold for notable discomfort, as only one individual was affected at that concentration. The 3 ppm point-of-departure was divided by an intraspecies uncertainty factor of 3, because response to sensory irritation is not expected to vary greatly among individuals (NRC 2001). A factor of 3 was considered sufficient because the effect of slight irritation is below the definition of AEGL-1. In addition, an intraspecies uncertainty factor of 3 was used to derive AEGL values for the related compounds HCl and HF, which have the same mode of action as HBr (NRC 2004). It is reasonable to use the same uncertainty factors for a class of chemicals whose mode of action is the same. Finally, the uncertainty factor used to derive the AEGL-1 values for HBr is believed to be protective of asthmatic individuals on the basis of comparison of the AEGL-1 value for HBr (1.0 ppm) with the AEGL-1 value for HCl (1.8 Acute Exposure Guideline Levels ppm); the latter is based on a no-effect level for irritation in exercising asthmatics. There is evidence that HBr is of similar toxicity to HCl; thus, the lower AEGL-1 values for HBr are considered to be protective of asthmatics on the basis of data on HCl. Because irritation depends on concentration rather than time, and adaptation to slight irritation occurs (Dalton 2001), 1.0 ppm was used for all of the AEGL-1 exposure durations (see Table 8-8). Derivation of the AEGL-1 values for HBr are presented in Appendixes A and D, and a category plot of the toxicity data for HBr in relation to AEGL values is presented in Appendix B. Although the AEGL-1 values for HBr are based on data presented in a secondary source, the values obtained from the data are supported by comparison with the related compounds HF and HCl. The AEGL-1 values for HF (1.0 ppm) and HCl (1.8 ppm) are equal to or higher than the values obtained for HBr using data from Connecticut State Department of Health (unpublished data, 1955, as cited in ACGIH 2002). Thus, if AEGL-1 values for HBr were obtained by analogy to these related compounds, the same or higher AEGL-1 values would be derived.”

The following justification for the HCl AEGL-1 values is an excerpt from the Subcommittee on Acute Exposure Guideline Levels (2004) [135].

“Because appropriate human data exist for exposure to HCl, they were used to identify AEGL-1 values. Exposure to HCl at 1.8 ppm for 45 min resulted in a no-observed-adverse-effect level (NOAEL) in 10 exercising young adult asthmatic subjects (Stevens et al. 1992). Because exercise will increase HCl uptake and exacerbate irritation, those asthmatic subjects are considered a sensitive subpopulation. Therefore, because the test subjects were a sensitive subpopulation and the end point was essentially a no-effect level, no uncertainty factor (UF) was applied to account for sensitive human subpopulations. Adequate human data were available, so no UF was applied for animal to human extrapolation. The no-effect level was held constant across the 10- and 30-

min and 1-, 4-, and 8-h exposure time points. That approach was considered appropriate because mild irritant effects generally do not vary greatly over time, and the end point of a no-effect level in a sensitive population is inherently conservative.”

The following justification for the HCN AEGL-1 values is an excerpt from the Subcommittee on Acute Exposure Guideline Levels (2002) [136].

“The AEGL-1 is based on monitoring studies in which the preponderance of data as a weight-of-evidence consideration indicates that an 8-h exposure to 1 ppm would be without adverse effects for the general population...The AEGL-1 was derived from a consideration of the dose-response data, which were obtained from all of the monitoring studies and subsequently time scaled to the shorter exposure durations. Although the exposures were of chronic duration in the monitoring studies, they represent the best available human data. Symptoms observed during chronic exposures should represent the greatest potential response. An 8-h exposure duration was selected as the basis for AEGL development. Mild headache is a symptom of exposure that meets the definition of an AEGL-1. Dividing the 8-h concentration of 5 ppm of the Grabois (1954), Hardy et al. (1950), or Maehly and Swensson (1970) study by an intraspecies uncertainty factor (UF) of 3 or dividing the 1-h concentration of 8 ppm of the El Ghawabi et al. (1975) study by an intraspecies UF of 3 results in very similar AEGL-1 values. The resulting 8-h value of 1.7 ppm is also similar to the 8-h no-effect concentration of 1 ppm in the Leeson et al. (1990) study, where no UF was applied. UFs are generally applied to the highest NOAELs or lowest LOAELs. A UF was not applied to the Leeson et al. (1990) study because it was the lowest NOAEL. No specific susceptible populations were identified during numerous occupational monitoring studies or during the clinical use of nitroprusside solutions to control hypertension. Thus, potential differences in susceptibility among humans are not expected to exceed 3-fold. All individuals, including infants, possess large amounts of the cyanide detoxifying enzyme rhodanese (as well as other detoxifying enzymes) and normally have adequate amounts of sulfur-containing compounds. The 8-h no-effect mean geometric concentration of 1 ppm (with excursions up to 6 ppm) from the Leeson et al. (1990) study was used as the basis for time scaling the AEGL-1 values. This study was chosen because it was well conducted: all workers had full medical examinations and routine blood tests, including measurements of blood cyanide and carboxyhemoglobin. Atmospheric HCN concentrations were monitored in the plant several times during the year. Because of the extrapolation from a long-term exposure, the 8-h value of 1 ppm was time scaled to the other exposure durations using the relationship $C_3 \times t = k$ where $k = 480 \text{ ppm} \cdot \text{min}$. In order to stay below the highest measured concentration from personal samplers, at 3.3 ppm in the Leeson et al. (1990) study, the 10-min value was set equal to the 30-min value.”

The following justification for the HF AEGL-1 values is an excerpt from the Subcommittee on Acute Exposure Guideline Levels (2004) [135].

“The AEGL-1 was based on an exposure at 3 parts per million (ppm) (range, 0.85-2.93 ppm) for 1 hour (h), which was the threshold for pulmonary inflammation, as evidenced by an increase in the percentage of several inflammatory parameters such as CD3 cells and myeloperoxidase in the bronchoalveolar lavage fluid of 20 healthy exercising adult subjects (Lund et al. 1999). There were no increases in neutrophils, eosinophils, protein, or methyl histamine at this or the next higher average exposure concentration of 4.7 ppm (range, 3.05-6.34 ppm). There were no changes in lung function and only minor symptoms of irritation at that concentration (Lund et al. 1997). Although healthy adults were tested, several individuals had increased immune factors, indicating atopy. The 3-ppm concentration was divided by an intraspecies uncertainty factor (UF)

of 3 to protect susceptible individuals. Because there were no effects on respiratory parameters of healthy adults at concentrations up to 6.34 ppm in the Lund et al. (1997) study and at concentrations up to 8.1 ppm for 6 h/day (d) with repeated exposures in a supporting study (Largent 1960, 1961), the calculated AEGL-1 values will be protective of asthmatic individuals. Although the Lund et al. (1999) study duration was only 1 h, the longer exposures at higher concentrations in the supporting study (Largent 1960, 1961), and the fact that adaptation to mild sensory irritation occurs, support application of the 1-ppm concentration for up to 8 h.”

The following justification for the NH_3 AEGL-1 values is an excerpt from the Committee on Acute Exposure Guideline Levels (2008) [137].

“Humans experience either faint or no irritation after exposure to ammonia at 30 ppm for 10 min (MacEwen et al. 1970); therefore, 30 ppm was used to derive AEGL-1 values. An interspecies uncertainty factor is not applied to these data because the AEGL value is based on human data. An intraspecies uncertainty factor of 1 was selected because ammonia is efficiently scrubbed in the upper respiratory tract, and if irritation occurs, it would be confined to the nasal cavity (and possibly the eyes). Nonatopic and atopic subjects, including asthmatics, responded similarly in a nasal airway resistance test when 100 ppm of ammonia was introduced into each nostril for up to 30 s (McLean et al. 1979); therefore, asthmatic individuals are not expected to respond differently than non-asthmatic individuals. Exercising subjects showed only a clinically nonsignificant decrease in pulmonary function after exposure to higher concentrations of ammonia (Cole et al. 1977); therefore, exercise is not expected to cause an appreciable difference in effects experienced during exposure to AEGL-1 concentrations. The same value is proposed for 5, 30, 60, 240, and 480 min, because any effects that occur are not expected to become more severe with duration of exposure because adaptation occurs during prolonged exposure. AEGL-1 values are summarized in Table 2-9. The AEGL-1 value of 30 ppm for all time points is supported by observations that humans reported similar intensities of response after exposure to 50 ppm for 10 min to 2 h (MacEwen et al. 1970; Verberk 1977).”

The following justification for the NO_2 AEGL-1 values is an excerpt from the Committee on Acute Exposure Guideline Levels (2012) [138].

“AEGL values were based on studies of NO_2 , the predominant form of the nitrogen oxides, and values are considered applicable to all nitrogen oxides. Values for N_2O_4 in units of ppm have been calculated on a molar basis. Because conversion to NO_2 is expected to occur in the atmosphere, and because NO_2 is more toxic than NO , the AEGL values for NO_2 are recommended for use with emergency planning for NO . The National Advisory Committee recognizes, however, that short-term exposures to NO below 80 ppm should not constitute a health hazard.... For AEGL-1, a concentration of 0.5 ppm was adopted for all time points. Although the response of asthmatics to NO_2 is variable, asthmatics were identified as a potentially susceptible population. The evidence indicates that some asthmatics exposed to NO_2 at 0.3-0.5 ppm might respond with either subjective symptoms or slight changes in pulmonary function that are not clinically significant. In contrast, some asthmatics did not respond to NO_2 at concentrations of 0.5-4 ppm. Because of the weight of evidence, the study by Kerr et al. (1978, 1979) was considered the most appropriate for derivation of AEGL-1 values. They reported that 7/13 asthmatics experienced slight burning of the eyes, slight headache, and chest tightness or labored breathing with exercise when exposed at 0.5 ppm for 2 h; at this concentration, the odor of NO_2 was perceptible but the subjects became unaware of it after about 15 min. No changes in any pulmonary function tests were found immediately following the chamber exposure (Kerr et al. 1978, 1979). Therefore, 0.50 ppm was considered a

no-adverse-effect level for the asthmatic population. Since asthmatics are potentially the most susceptible population, no uncertainty factor was applied. Time scaling was not performed because adaptation to mild sensory irritation occurs. In addition, animal responses to NO₂ exposure have demonstrated a much greater dependence on concentration than on time; therefore, extending the 2-h concentration to 8 h should not exacerbate the human response.”

The following justification for the SO₂ AEGL-1 values is an excerpt from the Committee on Acute Exposure Guideline Levels (2010) [139].

“AEGL-1 values were based on the weight-of-evidence from human asthmatic data suggesting that 0.20 ppm may be a NOEL for bronchoconstriction in exercising asthmatics. No treatment-related effects were noted in asthmatics exposed to 0.2 ppm for 5 min (Linn et al. 1983b), 0.25 ppm for 10-40 min (Schacter et al. 1984), 0.25 ppm for 75 min (Roger et al. 1985), 0.5 ppm for 10-40 min (Schacter et al. 1984), or 0.5 ppm for 30 min (Jorres and Magnussen 1990). However, an increase in airway resistance (S_{Raw}) of 134-139% was observed in exercising asthmatics exposed to 0.25 ppm for 5 min (Bethel et al. 1985); the increase in S_{Raw} in this study, but not in the other studies, may be attributed to the lower relative humidity (36%) in the Bethel et al. (1985) study compared to the other studies (70-85%). No uncertainty factors were applied because the weight of evidence approach utilized studies from a sensitive human population, exercising asthmatics. The role of exposure duration to the magnitude of SO₂-induced bronchoconstriction in asthmatics appears to decrease with extended exposure. For example, asthmatics exposed to 0.75 ppm SO₂ for 3-h exhibited increases in S_{Raw} of 322% 10-min into exposure, 233% 20-min into the exposure, 26% 1-hr into the exposure, 5% 2-h into the exposure, and a decrease of 12% at the end of the 3-h exposure period. These data suggest that a major portion of the SO₂-induced bronchoconstriction occurs within 10-min and increases minimally or resolves beyond 10-min of exposure. Therefore, AEGL-1 values for SO₂ were held constant across all time points. Exposure to concentrations at the level of derived AEGL-1 values is expected to have no effect in healthy individuals, but the concentrations are consistent with the definition of AEGL-1 for asthmatic individuals.”

7.5. *Exposure Limit Distances*

Table 42 through Table 45 present the distances at which exposure limits are exceeded for the non-flaming scenarios.

Table 46 through Table 49 present the distances at which exposure limits are exceeded for the flaming scenarios. The furthest exposure limit distance produced for each scenario is highlighted in yellow.

Table 42. LFP non-flaming thermal runaway FDS simulation results for IDLH limits.

Non-Flaming LFP			IDLH Distances [m]						
Temperature [C]	Wind Speed [m/s]	Duration [hr]	HF	CO	CO ₂	NO ₂	HCl	HCN	Benzene
7	2	6	0.5 ^a	0	0	41.75	0	0	0
7	5	6	5	0	0	62.25	0	0	0
7	10	6	0	0	0	28.75	0	0	0
7	2	12	0.5 ^a	0	0	34.25	0	0	0
7	5	12	0	0	0	27.75	0	0	0
7	10	12	0	0	0	11.25	0	0	0
22	2	6	0.5 ^a	0	0	50.75	0	0	0
22	5	6	5.5	0	0	63.75	0	0	0
22	10	6	0	0	0	28.75	0	0	0
22	2	12	0.375 ^a	0	0	45.75	0	0	0
22	5	12	0	0	0	29.25	0	0	0
22	10	12	0	0	0	12.25	0	0	0
35	2	6	7.75	0	0	54.75	0	0	0
35	5	6	6.5	0	0	69.75	0	0	0
35	10	6	0	0	0	33.25	0	0	0
35	2	12	0.25 ^a	0	0	39.75	0	0	0
35	5	12	0	0	0	27.75	0	0	0
35	10	12	0	0	0	12.50	0	0	0

a) Distance was evaluated at the sides of the BESS unit, not downwind

Table 43. LFP non-flaming thermal runaway FDS simulation results for AEGL-1, ERPG-1, & TEEL-1 limits.

Non-Flaming LFP			AEGL-1, ERPG-1, & TEEL-1 Distances [m]						
Temperature [C]	Wind Speed [m/s]	Duration [hr]	HF	CO	CO ₂	NO ₂	HCl	HCN	Benzene
7	2	6	117.25	0	0	200+	62.25	18.75	9.25
7	5	6	165.75	2.625	0	200+	100.25	19.75	10
7	10	6	119.25	0	0	200+	57.25	9	3.75
7	2	12	103.25	0	0	200+	56.75	12.5	6
7	5	12	113.75	0	0	200+	54.25	8.25	3.25
7	10	12	71.75	0	0	200+	48.75	2.625	0
22	2	6	114.25	0	0	200+	71.75	23.25	11.75
22	5	6	168.25	3.75	0	200+	103.75	20.25	10.75
22	10	6	121.75	0	0	200+	56.75	9.5	4
22	2	12	115.75	0	0	200+	65.25	15.25	8
22	5	12	119.75	0	0	200+	58.75	9.25	4.25
22	10	12	74.75	0	0	200+	24.25	2.75	0
35	2	6	139.75	0	0	200+	75.75	27.25	15.25
35	5	6	168.25	4.5	0	200+	107.75	22.75	11.5
35	10	6	125.25	0	0	200+	63.75	10.25	4.5
35	2	12	103.25	0	0	200+	64.25	15.75	7
35	5	12	124.25	0	0	200+	57.75	9	11.5
35	10	12	77.25	0	0	200+	25.75	3.5	0

Table 44. NMC non-flaming thermal runaway FDS simulation results for IDLH limits.

Non-Flaming NMC			IDLH Distances [m]					
Temperature [C]	Wind Speed [m/s]	Duration [hr]	HF	CO	CO ₂	HCl	HCN	Benzene
7	2	0.5	0	0	0	0.375	0	0
7	5	0.5	0.25 ^a	15.25	0	42.25	0	0.25 ^a
7	10	0.5	0	20.25	0	75.75	0	0.25 ^a
7	2	2	0	0	0	0.25	0	0
7	5	2	0	8.25	0	27.75	0	0
7	10	2	0	2.625	0	14.25	0	0
22	2	0.5	0	0	0	0.375	0	0
22	5	0.5	0.25 ^a	17.75	0	48.75	0	0.25 ^a
22	10	0.5	0	21.25	0	81.25	0	0.25 ^a
22	2	2	0	0	0	11.75	0	0
22	5	2	0	9	0	31.25	0	0
22	10	2	0	3.5	0	15.75	0	0
35	2	0.5	0	0.25 ^a	0	0.375	0	0
35	5	0.5	0.25 ^a	21.75	0	54.75	0	0.25 ^a
35	10	0.5	0	22.25	0	80.75	0	0.25 ^a
35	2	2	0	0	0	14.25	0	0
35	5	2	0	9.75	0	34.75	0	0
35	10	2	0	3.5	0	16.75	0	0

a) Distance was evaluated at the sides of the BESS unit, not downwind

Table 45. NMC non-flaming thermal runaway FDS simulation results for AEGL-1, ERPG-1, & TEEL-1 limits.

Non-Flaming NMC			AEGL-1, ERPG-1, & TEEL-1 Distances [m]					
Temperature [C]	Wind Speed [m/s]	Duration [hr]	HF	CO	CO ₂	HCl	HCN	Benzene
7	2	0.5	0	0	0	30.5	0	0
7	5	0.5	73.75	72.75	0	200+	0	35.75
7	10	0.5	132.75	130.25	0	200+	0	62.25
7	2	2	17.75	17.25	0	112.75	0	3.75
7	5	2	69.25	65.75	0	200+	0	22.75
7	10	2	43.25	40.75	0	200+	0	12
22	2	0.5	0	0	0	24.75	0	0
22	5	0.5	85.25	83.75	0	200+	0	41.25
22	10	0.5	133.75	131.75	0	200+	0	65.75
22	2	2	22.75	21.75	0	144.75	0	9.25
22	5	2	76.25	72.75	0	200+	0	24.75
22	10	2	45.25	42.75	0	200+	0	12.5
35	2	0.5	0	0	0	35.25	0	0
35	5	0.5	95.25	93.75	0	200+	0	46.75
35	10	0.5	140.25	138.25	0	200+	0	69.75
35	2	2	30.25	29.25	0	156.75	0	13.75
35	5	2	81.25	78.25	0	200+	0	28.75
35	10	2	48.75	45.75	0	200+	0	12.5

Table 46. LFP flaming thermal runaway FDS simulation results for IDLH limits.

Flaming LFP			IDLH Distances [m]						
Temperature [C]	Wind Speed [m/s]	Duration [hr]	HF	CO	CO ₂	NO ₂	HCl	SO ₂	NH ₃
7	2	2	0	0	0	0	0	0	0
7	5	2	0.125 ^a	0	0	0	0	0	0
7	10	2	1 ^a	0	0	0.75 ^a	0	0	0
7	2	4	0	0	0	0	0	0	0
7	5	4	0.125 ^a	0	0	0	0	0	0
7	10	4	0.75 ^a	0	0	0.5 ^a	0	0	0
7	2	6	0	0	0	0	0	0	0
7	5	6	0	0	0	0	0	0	0
7	10	6	0.75 ^a	0	0	0.5 ^a	0	0	0
22	2	2	0	0	0	0	0	0	0
22	5	2	0.125 ^a	0	0	0	0	0	0
22	10	2	1.125 ^a	0	0	0.75 ^a	0	0	0
22	2	4	0	0	0	0	0	0	0
22	5	4	0.125 ^a	0	0	0	0	0	0
22	10	4	0.875 ^a	0	0	0.5 ^a	0	0	0
22	2	6	0	0	0	0	0	0	0
22	5	6	0.125 ^a	0	0	0	0	0	0
22	10	6	0.75 ^a	0	0	0	0	0	0
35	2	2	0	0	0	0	0	0	0
35	5	2	0.125 ^a	0	0	0	0	0	0
35	10	2	1.125 ^a	0	0	0.75 ^a	0	0	0
35	2	4	0	0	0	0	0	0	0
35	5	4	0.125 ^a	0	0	0	0	0	0
35	10	4	0.875 ^a	0	0	0.5 ^a	0	0	0
35	2	6	0	0	0	0	0	0	0
35	5	6	0.125 ^a	0	0	0	0	0	0
35	10	6	0.75 ^a	0	0	0.5 ^a	0	0	0

a) Distance was evaluated at the sides of the BESS unit, not downwind

Table 47. LFP flaming thermal runaway FDS simulation results for AEGL-1, ERPG-1, & TEEL-1 limits.

Flaming LFP			AEGL-1, ERPG-1, & TEEL-1 Distances [m]					
Temperature [C]	Wind Speed [m/s]	Duration [hr]	HF	CO	CO ₂	NO ₂	HCl	NH ₃
7	2	2	0	0	0	0	0	0
7	5	2	1.875	0	0	0	0	0
7	10	2	12.75	0	0	0	0	0
7	2	4	0	0	0	0	0	0
7	5	4	0.625	0	0	0	0	0
7	10	4	13.25	0	0	0	0	0
7	2	6	0	0	0	0	0	0
7	5	6	0.375	0	0	0	0	0
7	10	6	12.75	0	0	0	0	0
22	2	2	0	0	0	0	0	0
22	5	2	2	0	0	0	0	0
22	10	2	12.75	0	0	0	0	0
22	2	4	0	0	0	0	0	0
22	5	4	0.75	0	0	0	0	0
22	10	4	16.25	0	0	0	0	0
22	2	6	0	0	0	0	0	0
22	5	6	2.25	0	0	0	0	0
22	10	6	15.75	0	0	0	0	0
35	2	2	0	0	0	0	0	0
35	5	2	2	0	0	0	0	0
35	10	2	12.75	0	0	0.25	0	0
35	2	4	0	0	0	0	0	0
35	5	4	2	0	0	0	0	0
35	10	4	14.75	0	0	0	0	0
35	2	6	0	0	0	0	0	0
35	5	6	0.75	0	0	0	0	0
35	10	6	12.75	0	0	0	0	0

Table 48. NMC flaming thermal runaway FDS simulation results for IDLH limits.

Flaming NMC			IDLH Distances [m]								
Temp. [C]	Wind Speed [m/s]	Duration [hr]	HF	CO	CO ₂	NO ₂	HCl	HCN	HBr	SO ₂	Benzene
7	2	2	0	0	0	0	0	0	0	0	0
7	5	2	0	0	0	0	0	0	0	0	0
7	10	2	1 ^a	0	0	0.75 ^a	0	0	0	0	0.5 ^a
7	2	4	0	0	0	0	0	0	0	0	0
7	5	4	0	0	0	0	0	0	0	0	0
7	10	4	0.75 ^a	0	0	0.5 ^a	0	0	0	0	0.375 ^a
7	2	6	0	0	0	0	0	0	0	0	0
7	5	6	0	0	0	0	0	0	0	0	0
7	10	6	0.625 ^a	0	0	0.5 ^a	0	0	0	0	0
22	2	2	0	0	0	0	0	0	0	0	0
22	5	2	0	0	0	0	0	0	0	0	0
22	10	2	1 ^a	0	0	0.5 ^a	0	0	0	0	0.375 ^a
22	2	4	0	0	0	0	0	0	0	0	0
22	5	4	0	0	0	0	0	0	0	0	0
22	10	4	0.625 ^a	0	0	0.5 ^a	0	0	0	0	0.375 ^a
22	2	6	0	0	0	0	0	0	0	0	0
22	5	6	0	0	0	0	0	0	0	0	0
22	10	6	0.625 ^a	0	0	0.5 ^a	0	0	0	0	0.375 ^a
35	2	2	0	0	0	0	0	0	0	0	0
35	5	2	0	0	0	0	0	0	0	0	0
35	10	2	1 ^a	0	0	0.75 ^a	0	0	0	0.375 ^a	0.375 ^a
35	2	4	0	0	0	0	0	0	0	0	0
35	5	4	0	0	0	0	0	0	0	0	0
35	10	4	0.625 ^a	0	0	0.5 ^a	0	0	0	0	0
35	2	6	0	0	0	0	0	0	0	0	0
35	5	6	0	0	0	0	0	0	0	0	0
35	10	6	0.625 ^a	0	0	0.5 ^a	0	0	0	0	0

a) Distance was evaluated at the sides of the BESS unit, not downwind

Table 49. NMC flaming thermal runaway FDS simulation results for AEGL-1, ERPG-1, & TEEL-1 limits.

Flaming NMC			AEGL-1, ERPG-1, & TEEL-1 Distances [m]								
Temp. [C]	Wind Speed [m/s]	Duration [hr]	HF	CO	CO ₂	NO ₂	HCl	HCN	HBr	SO ₂	Benzene
7	2	2	0	0	0	0	0	0	0	0	0
7	5	2	0	0	0	0	0	0	0	0	0
7	10	2	12	0	0	0.35	0	0	0	13.75	0
7	2	4	0	0	0	0	0	0	0	0	0
7	5	4	0	0	0	0	0	0	0	0	0
7	10	4	3.25	0	0	0	0	0	0	12.75	0
7	2	6	0	0	0	0	0	0	0	0	0
7	5	6	0	0	0	0	0	0	0	0	0
7	10	6	5	0	0	0	0	0	0	11.25	0
22	2	2	0	0	0	0	0	0	0	0	0
22	5	2	0	0	0	0	0	0	0	0	0
22	10	2	12.5	0	0	0.25	0	0	0	14.25	0
22	2	4	0	0	0	0	0	0	0	0	0
22	5	4	0	0	0	0	0	0	0	0	0
22	10	4	3.25	0	0	0	0	0	0	12.5	0
22	2	6	0	0	0	0	0	0	0	0	0
22	5	6	0	0	0	0	0	0	0	0	0
22	10	6	4.5	0	0	0	0	0	0	11.75	0
35	2	2	0	0	0	0	0	0	0	0	0
35	5	2	0	0	0	0	0	0	0	0.375	0
35	10	2	12.5	0	0	0.375	0	0	0	14.25	0
35	2	4	0	0	0	0	0	0	0	0	0
35	5	4	0	0	0	0	0	0	0	0	0
35	10	4	3.5	0	0	0	0	0	0	12.75	0
35	2	6	0	0	0	0	0	0	0	0	0
35	5	6	0	0	0	0	0	0	0	0	0
35	10	6	10.75	0	0	0	0	0	0	14.75	0

Table 50. AERMOD simulation results for AEGL-1, ERPG-1, & TEEL-1 limits.

Scenario			AEGL-1, ERPG-1, & TEEL-1 Safety Distances [m]									
Cell Chemistry	Thermal Runaway Conditions	Duration [hr]	HF	CO	CO2	NO2	HCl	HCN	HBr	SO2	Benzene	NH3
LFP	Flaming	4	83	0	0	0	0	-	-	0	-	0
LFP	Non-flaming	6	61	0	0	322	22	0	-	-	0	-
NMC	Flaming	4	50	0	0	12	0	0	0	62	0	-
NMC	Non-flaming	0.5	22	56	0	-	418	0	-	-	21	-

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