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Simulation of Thermal Propagation in a Large Battery Module

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Executive Summary

A multi-physics thermal propagation model of a battery module, consisting of 507 cylindrical 18650 cells, was built using a commercial software. The model incorporated an empirical method for self-heating in battery cells, a 3-Dimentional (3-D) Finite Element method (FEM) for simulating thermal propagation in solid materials, and sub-models for thermal convection and radiation. Simulations reveal the significance of thermal convection in thermal propagation. The model agreed well with the experimental data until around half of the cells entered thermal runaway (around 22 minutes), with an observed overprediction of heat release afterward. This overprediction might be attributed to inaccuracies in thermal convection and the omission of burning vented gases and solid particles.

Keywords: lithium-ion battery, thermal runaway, multi-physics simulations, cost-efficient, large-scale experiments.

1 Introduction

Battery thermal runaway poses significant challenges to various sectors of electrification including electric vehicles, battery energy storage systems, battery manufacturing, second use and recycling. Therefore, understanding and estimating battery thermal runaway is crucial for a smooth transition to an electrified society.

Battery thermal runaway is a complex, multi-physics and multi-scale process, presenting challenges in developing detailed models due to the abundance of physical and chemical phenomena. These phenomena include electrochemical reactions within the cell, self-heating of the cell, exothermic reactions of decomposition of battery components, endothermic reactions such as melting of separator and aluminum, evaporation of organic solvents in electrolyte, venting of flammable and toxic gas, ejection of aerosols (solid particles and liquid droplets), burning of gas and particles, heat transfer, heat radiation, and so on [1]. Multi-physics simulation is a cost-efficient approach in simulating battery thermal runaway. However, due to the complexity of large-scale battery thermal runaway behaviors, it is important to calibrate models with experiments.

This work introduces a cost-efficient thermal runaway model for a sizable battery module comprising 507 cylindrical cells (18650 format) with Nickel-Cobalt-Manganese (NCM) chemistry, offering a valuable comparison with large-scale experiments. The term "cost-efficient" denotes that the calibrated model facilitates exploration within the design space through parametric studies, diminishing the reliance on numerous expensive experiments. Notably, this simple battery thermal propagation model features a short runtime even for large battery module meaning low computational cost. The advantages and limitations of this methodology are discussed.

2 Experimental setup

The cells utilized in the large-scale fire test were cylindrical 18650, NCM type cells, configured into a module enclosed within a casing measuring 440 x 358 x 174 mm and possessing a total weight, including cells, of 36.5 kg. A total of 507 cells were configured in a 13S39P arrangement. The assembly consisted of 13 strings arranged in series, with each string comprising 39 cells in parallel. The configuration was divided into two subassemblies: a bottom level featuring nine serially connected strings, and a top level with four such strings, incorporating a battery management system (BMS) and electronics. Thin Mylar® film enveloped the cell assemblies in each level to ensure electrical insulation, with a 2 mm steel plate supporting the upper level. The cells had a nominal capacity of 100 Ah (approximately 2.55 Ah per cell) and operated at a nominal voltage of 46.8 V, resulting in a total module energy of 4 680 Wh.

During the large-scale fire test, designed to replicate a battery energy storage system, the module was situated within a rack comprising 11 dummy modules filled with sand (not containing any battery cells). The rack was configured with 4 modules vertically and 3 modules horizontally. The module under examination (referred to as the live module) occupied the central position, located second from the bottom (refer to Fig. 1). The live module was equipped with nine internal temperature sensors (thermocouples) and six additional thermocouples were placed on the exterior of the module. The internal thermocouples were attached to the cells using non-conducting tape. Data was sampled at a frequency of 1 Hz. To facilitate the capture of all battery vent gases, the test setup was enveloped with non-combustible boards.

The experiments were conducted in an indoor fire laboratory, allowing for precise measurements of gas emissions and the calculation of the heat release rate (HRR). Details regarding the equations and instrumentation applied for computing the HRR can be referenced in Dahlberg [2]. For safety considerations, spark igniters were positioned in front of the test setup to promptly ignite any flammable gases released, thus preventing the accumulation of such gases. Thermal runaway was initiated using an external propane burner featuring a Sievert Pro 86 nozzle with a 22 mm diameter, a working pressure of 2 bar, and a heating output of 3.1 kW. A hood connected to the exhaust duct collected combustible gases. The exhaust duct was equipped with flue gas reduction and water purification systems, integrated into the fire hall to minimize the environmental impact of fire testing. Additional details about the test setup can be found in Bisschop et al. [3]

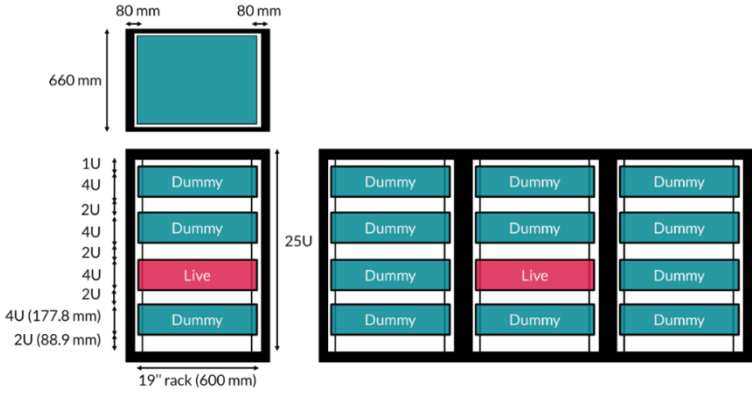

Figure 1: Illustration of test setup, the live module is shown in red [3].

3 Numerical method and setup

The objective of this study is to present a multi-physics model designed for investigating thermal runaway in large battery systems. The following parts outline the numerical methodology, and the setup employed for simulations. The simulations were conducted using a commercial multi-physics software GT-SUITE version-2021, developed by Gamma Technologies [4].
The governing equation employed to calculate the temperature during TR based on energy balance is written as follows:

$$\rho_{jr} c_{p,jr} \frac{dT}{dt} - \nabla \cdot (k \nabla T) = \frac{\dot{Q}_{gen}}{V_{jr}} + \frac{\dot{Q}_{conv}}{V_{jr}} + \frac{\dot{Q}_{rad}}{V_{jr}}, \quad (1)$$

where ρ_{jr}, V_{jr} , $c_{p,jr}$ and k represent the density, volume, specific heat capacity and thermal conductivity of the jelly roll, respectively. $\dot{Q}_{gen}$ denotes the internal heat generation rate of cell during TR, including heat produced by the thermal decomposition reactions of battery components, such as the cathode, electrolyte, separator, anode, binder, and joule heat due to internal short circuits. The heat produced by thermal decomposition reactions is often computed using multi-step kinetic reaction mechanisms following the Arrhenius equation. Alternatively, the heat production from chemical reactions can be measured by ARC or DSC. The joule heat due to internal short circuits can be calculated using the electric equivalent method and calibrated using experimental data. The empirical method is applied to initiate TR by applying a steady heat generation rate over a short period [5]. This reduces computational costs and addresses the absence of cell-level experimental data. Specifically, TR is triggered when the average cell temperature reaches an onset temperature T_{onset}. $\dot{Q}_{conv}$ and $\dot{Q}_{rad}$ represent the heat transfer rate between the battery and the surroundings through convection and thermal radiation, respectively. They are calculated as follows:

$$\dot{Q}_{conv} = -hA\left(T_{jr} - T_{int}\right), \quad (2)$$

$$\dot{Q}_{rad} = -\varepsilon \sigma A\left(T_{jr}^4 - T_{jr,n}^4\right), \quad (3)$$

where h is the convective heat transfer coefficent; T_{jr} is the jelly roll temperature; $T_{jr,n}$ is the neighbouring jelly roll temperature; T_{inter} is the internal gas temeperature obtained in the expeirments (see Fig. 4); ε=0.9 is the surface emissivity of the cell; σ= 5.67·10^{-8} W m^{-2} K^{-4} is the Stefan-Boltzman constant. The model constants and material properties used in this work are listed in Table 1. Note that the plastic holder used in the battery module is a thermoplastic polymer known as acrylonitrile butadiene styrene (ABS). The material properties of the steel plate are obtained from the standard GT-Suite material library [4].

Table 1 Parameters used for solving Equations (1-3).

Parameter	Value	Unit	Source
$c_{p,ABS}$	1 990	J kg^{-1} K^{-1}	matweb.com
$c_{p,jr}$	830	J kg^{-1} K^{-1}	Not available
k_{ABS}	0.136	W m^{-1} K^{-1}	matweb.com
k_{jr}	(0.2, 0.2, 30.4)*	W m^{-1} K^{-1}	[6]
h	10	W m^{-2} K^{-1}	Not available
h_{jr-ph}	800	W m^{-2} K^{-1}	Not available
h_{jr-sp}	2 000	W m^{-2} K^{-1}	Not available
$\dot{Q}_{gen}$	3.5	kW	Calibrated
$t_{dur,TR}$	10	s	Not available
T_{onset}	135	°C	Calibrated
ρ_{abs}	1 070	kg m^{-3}	matweb.com
ρ_{jr}	2 800**	kg m^{-3}	Not available

* The thermal conductivity of the jelly roll is anisotropic and has different values in cylindrical coordinates (r, Φ, z).

**This value is calculated based on an 18650-type cell with a weight of 47 g.

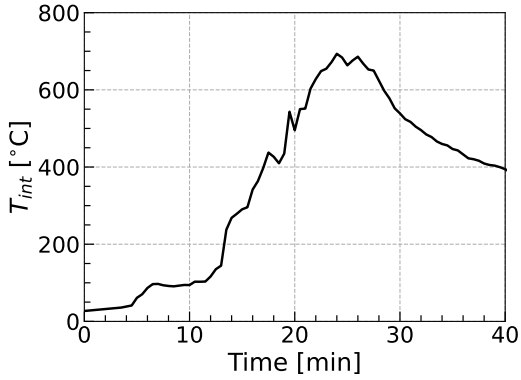

Figure 2: Measured internal gas temperature profile averaged from two tests [3].

This thermal runaway model with a brief runtime incorporates a 3-D FEM thermal model and an empirical approach for thermal runaway simulation [5]. Given the inherent complexity of battery thermal runaway processes, in-depth simulations are still in their early stages, and demand significant computational resources.

The 3-D thermal propagation model incorporated the battery cells, plastic holders, and steel plate, as illustrated in Fig. 3, while excluding BMS electronics, plastic enclosures around the lower and upper level of battery assemblies, and steel casing. Thermal runaway was initiated by applying a constant heat source of 400 W to a cell in the same position as the experiment until a stable thermal propagation was achieved. The stable thermal propagation was defined as the point when nine cells reached thermal runaway.

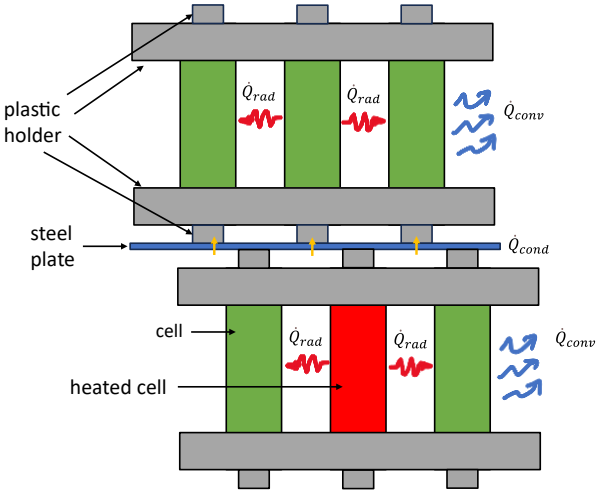

Figure 3: 2-dimentional illustration of the heat transfer pathways within battery cells arranged on two levels.

The large-scale thermal propagation model was built in a step-by-step fashion to save computational time and efforts. First, a small-scale model containing 78 cylindrical cells was constructed, debugged, and calibrated with experimental data. Subsequently, the model was expanded to a large-scale version containing 507 cylindrical cells. The large-scale model consisted of 200 905 finite elements with a cell size ranging from 2 to 10 mm. A single simulation, covering a duration of 40 minutes, required 2 hours and 47 minutes of CPU time on a laptop equipped with an Intel Core i7-7820 HQ CPU and 32 GB RAM. The initial temperature for the battery components in the simulations was set at 300 K.

4 Results and discussions

The evolution of temperature distribution within the battery module is shown in Fig. 4. Notably, thermal runaway is initiated in the cells of the lower level before spreading to those in the upper level. Among the upper-level cells, those at the boundaries experience thermal runaway first, followed by those in the middle of the module. This pattern can be attributed to the elevated ambient gas temperature employed in the model, emphasizing the thermal convection as the primary pathway for thermal propagation. A closer examination

of the thermal propagation pathways for a cell positioned in the lower right corner of the battery pack is done. Thermal convection plays a predominant role in heating the battery cell, contributing to approximately 60 % of the total heat transfer until the cell undergoes thermal runaway. The simulation indicates that thermal radiation accounts for about 26 % of the overall heat transfer, while conduction contributes to the remaining 14 %.

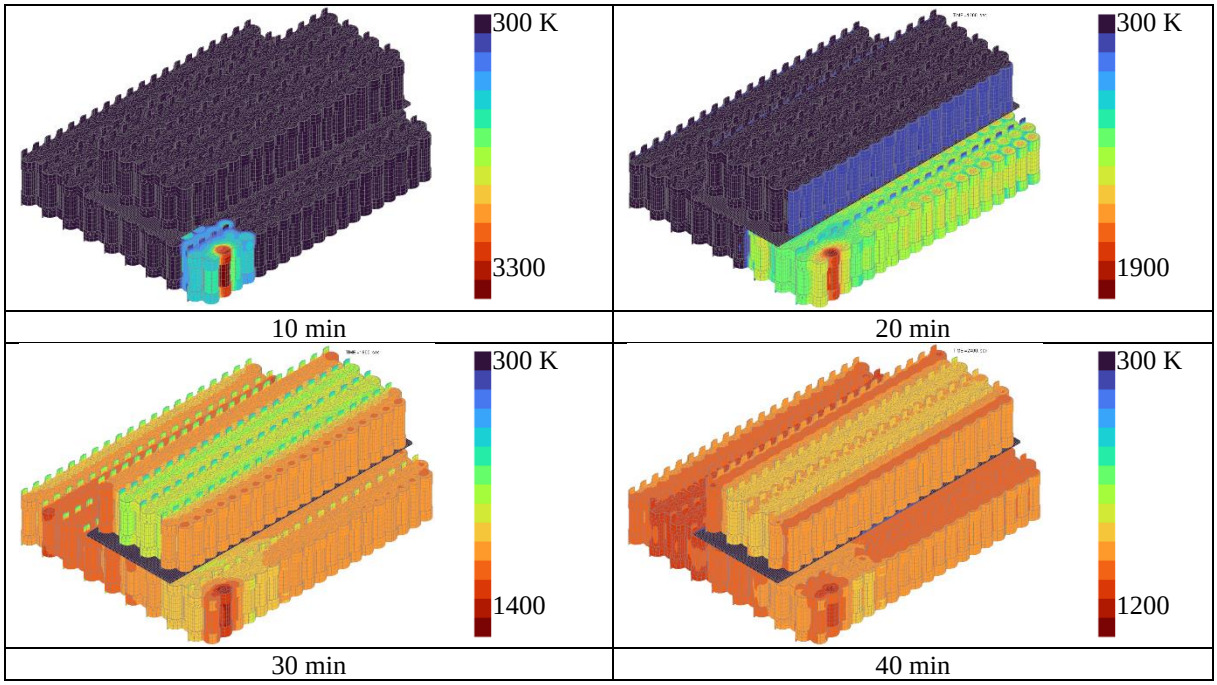

Figure 4: The evolution of temperature distribution within the battery module at different time instants.

A comparison between the measured total heat release and the computed number of cells experiencing thermal runaway is shown in Fig. 5. We assume that the number of cells experiencing thermal runaway is in proportion to the heat release applied. The comparison shows that the computed curve aligns well with the experimental one until approximately 22 minutes, when about half of the cells have entered thermal runaway. After that, the computed curve shows a faster growth compared to the experimental curve. It is worth noting that the heat release curve measures the burning of vented battery hot matters (gases and particles).

There are several reasons for this observed discrepancy. First, the multi-physics model, which employs a constant convective heat transfer coefficient can be improved. Theoretical calculations by Kong et al. [7] demonstrate that the convective heat transfer coefficient h can vary significantly, i.e., from 1.11 to 51.63 W m^{-2} K^{-1}, by varying ambient temperature from 260 to 320 K and ambient air velocity from 0.01 to 5 m/s. Second, the combustion involves the partially premixed turbulent burning of battery vent gases [8] and burning of ejected particles from cathode and anode materials. The neglection of these burning processes may contribute to the steeper increase in the computed curve. Nevertheless, the multi-physics battery thermal propagation model performs well in the initial and intermediate time range of thermal propagation which is critical for mitigating thermal runaway. This suggests that the model is promising and could be used for designing safer batteries. However, it requires careful calibration through comparisons with experiments to quantify thermal propagation pathways, including conduction, convection, and radiation.

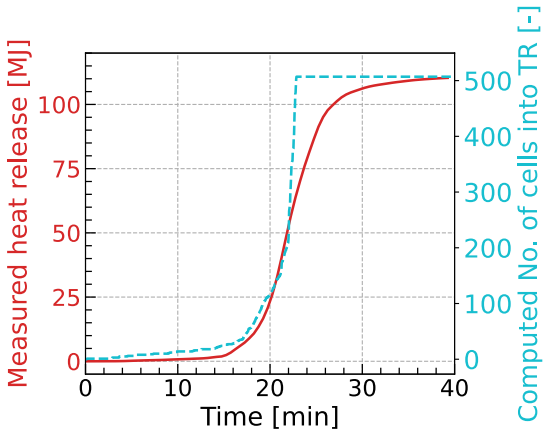

Figure 5: Comparison between experimental heat release and computed number of cells going into thermal runaway.

5 Conclusions

A multi-physics thermal propagation model for a battery module containing 507 cells of 18650 type was built using commercial software. The battery thermal propagation model incorporates an empirical method to simulate self-heating in battery cells, a 3-D FEM model for simulating thermal propagation in solid materials, and sub-models for thermal convection and radiation. The measured temperature inside the battery module was used to evaluate the thermal convection. The simulations showed the significant role of thermal convection in the battery module's thermal propagation. Quantitative comparison was made between the number of cells entering TR and the experimentally measured heat release, with the assumption that the number of cells into TR was proportional to the heat release. The model demonstrated good agreement with the experimental data until approximately half of the cells entered thermal runaway, around the 22-minute mark. Thereafter the model tended to over-predict the heat released. Potential reasons for this overprediction include a potential overestimation of thermal convection, and the exclusion of burning processes for vented matters such as gases and solid particles. Despite these limitations, the battery thermal propagation model proves particularly valuable for estimating thermal runaway in the early and intermediate stages. It is an effective tool for exploring design variations through parametric studies.

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Presenter Biography

With a solid background and extensive experience in simulations using numerical tools, particularly Computational Fluid Dynamics (CFD), encompassing areas such as chemical kinetics, combustion, multi-phase flow, turbulence, and more. Proficient in both commercial and open-source CFD codes, as well as commercial multi-physics codes and open-source data analysis tools like Python. Holds a PhD in thermal and fluid dynamics awarded in 2014 from Chalmers University of Technology. Possesses a keen interest in combustible dust safety and occupational safety. Considerable experience in battery fire and thermal propagation simulations.