Modelling thermal runaway initiation and propagation for batteries in dwellings to evaluate tenability conditions

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BRANDFORSK 2022:6



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This report constitutes a final working manuscript for the headlined project. The official project report, to which reference should be made, can be found on the RISE's website

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Abstract

Modelling thermal runaway initiation and propagation for batteries in dwellings to evaluate tenability conditions

Thermal propagation is one of the major challenges when batteries will be used in dwellings in large scale. It means the exothermic reactions in the cell are out of control and can lead to a fast release of flammable and toxic gases. In a system involving a large number of cells, thermal runaway can rapidly propagate from one battery cell to the whole system, which means substantial fire and explosion risks, an event that is important to mitigate and prevent. Multi-physics simulations together with full-scale testing is a cost-effective method for designing safer batteries. This project aims at simulating thermal runaway initiation and propagation using a multi-physics commercial software GT-Suite.

A battery thermal runaway model containing 12 prismatic cells based on 3-D Finite Element approach was built using GT-Suite. The computed thermal runaway time instants versus thermal runaway cell number were compared with full-scale experimental data with reasonable agreement. Quantitative sensitivity study on the model input parameters and model space and time resolutions on the computed start time instant and time duration of thermal runaway were performed. The thermal runaway model was then extended with an electric equivalent sub-model to simulate the short circuit. With the electrical model acting as the input to the thermal model, the most interesting output of the simulation is the change in temperature of the cells, dependent on the current in the cells, with respect to time. The current is determined by the value of the external resistance through which the short takes place and the voltage level of the battery pack. The obtained results from the above short circuit simulations can only be used as a starting point and not as absolute values for neither triggering the thermal model nor for accurately simulating a battery under an electrical load. Furthermore, GT-Suite was applied to simulate the gas dispersion inside a room. A comparative study of the dispersion of toxic gases during thermal runaway, utilising an arbitrary release of HCN to represent the battery gases, in a small compartment with natural ventilation was investigated and the results compared the same situation simulated in FDS. The pipe based modelling supported by GT-Suite has limited applicability and overestimated the concentrations close to the ceiling whereas the lateral concentrations where underestimated.

The multi-physics model for battery thermal runaway process is promising and worth to be applied with care for designing safer batteries in combination with full-scale testing.

Key words: battery thermal runaway, multi-physics simulation, short circuit, dwelling, gas dispersion.

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Preface

The Authors are grateful for the financial support from Swedish Fire Research Board (BRANDFORSK) under contract 322-001 "Modelling thermal runaway initiation and propagation for batteries in dwellings to evaluate tenability conditions" which made this work possible. We have also benefitted from scientific input from an advisory group consisting of people with different backgrounds:

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Sammanfattning

Värmetransport som uppkommer efter en termisk rusning i ett batteri är en av de stora utmaningarna när batterimoduler börjar användas i bostäder i stor skala. Det betyder att den möjliga exoterma reaktionen i cellen är utom kontroll vilket kan leda till ett snabbt utsläpp av brandfarliga och giftiga gaser i närområdet av batteriet eller batterimodulen. I en batterimodul som innefattar ett stort antal celler kan en termisk rusning snabbt spridas från en battericell till ett stort antal celler relativt snabbt, vilket innebär en betydande brand- och explosionsrisk. Det är viktigt att förebygga och fördröja sådana katastrofala spridningshändelser. En fördröjning gör att färre celler samtidigt genererar värme och gaser och därmed minskar risken för ytterligare spridning. Multifysiksimuleringar tillsammans med fullskaliga försök kan vara ett kostnadseffektivt sätt att designa säkrare batterier. Detta projekt syftar till att simulera hur en termisk rusning fortplantas med hjälp av en kommersiell multifysikprogramvara GT-Suite.

En termisk modell enligt 3-D Finite Elementmetoden (FEM) för batterimodulen skapades i GT-Suite, modellen innehåller 12 prismatiska celler. I modellen kunde den termiska rusningen predikteras och jämföras med experimentella data, modellen gav en bra rimlig överensstämmelse. Flera kvantitativa känslighetsstudier med de olika parametrarna inklusive geometriska och beräkningstekniska parametrar studerades och varaktigheten för hela spridning kunde jämföras. Modellen för den termiska rusningen utökades sedan med en elektrisk kretsmodell för att simulera en extern kortslutning. Med en kombination av elektriska och den termiska modellen, kan temperaturförändringen i cellerna, som beror på strömmen genom cellen, beräknas som funktion av tiden. Strömmen bestäms av värdet på det externa motståndet genom vilket kortslutningen sker och batteripaketets spänningsnivå. De erhållna resultaten från kortslutningssimuleringarna ovan kan endast användas som en startpunkt och inte som absoluta värden för att varken trigga den termiska modellen eller för att noggrant simulera ett batteri under en elektrisk belastning. En av anledningarna till det begränsade resultatet är att uppmätta data över cellerna och modulernas respons behövs för modellerna.

Vidare användes GT-Suite för att simulera gasspridningen i ett rum. En uppskattning av spridningen av en toxisk gas, där resultaten illustreras för HCN, med naturlig ventilation undersöktes och resultaten jämfördes med samma situation simulerad med FDS. GT-Suite använder en förenklad modell som bygger på flödet genom tunna rör och har därmed begränsad tillämpbarhet. Modellen överskattade koncentrationerna av HCN kraftigt nära taket medan de laterala koncentrationerna underskattades.

Multifysikmodellen för propagering av en termisk rusning i en modell är mycket lovande och värd att tillämpas vid design av säkrare batterier men då endast i kombination med försök där kalibrering av indata och validering av modellen blir en naturlig del.

Nyckelord: termisk rusning, multifysik, simulering, kortslutning, bostad, toxicitet, gasspridning.

1 Introduction

Energy and electricity are high on the agenda for many people now, especially in the light of recent changes in electricity price. There has already been an increased interest for using different energy storages to make better use of locally produced energy sources such as wind and solar energy but also to be able to charge when prices are low and use the stored electricity when prices are higher. The recent price changes might increase this further.

Batteries are useful for storing energy for short time periods like from one day to the next. The dominant battery type today is lithium-ion batteries due to their good performance in terms of energy density and long lifetime and are today used in many applications such as electric vehicles and handheld tools. Lithium-ion batteries have however a safety drawback as they contain a flammable electrolyte and have the potential to end up in a thermal runaway, a state of rapid self-heating. This is something that is of concern especially if these capacities become larger and are to be used in peoples home etc. and is also a concern for the rescue services. Test methods have begun to be developed for ensuring that if a thermal runaway happens then it shall not propagate to neighbouring cells. Testing is however expensive and resource demanding and the ability to use computer models for evaluating the potential for thermal propagation is therefore an important topic.

Modelling thermal runaway and thermal runaway propagation comprises of two different aspects, the risk of thermal runaway happening in a cell, e.g. due to different kinds of abuse, and the risk that thermal runaway is spread to adjacent cells or modules. The two aspects are connected as the spreading also involves thermal runaway initiation in adjacent cells/modules, but this initiation might in many cases be modelled in a simpler way when evaluating spread.

There are many different battery modelling tools available. The primary goal of battery modelling is normally to predict and optimise battery performance, typically in terms of charge/discharge characteristics but also for risk assessments. Over the past few decades, many battery models have been developed for different applications that differ in complexity, input parameters, available outputs and overall accuracy.

Rapidly discharging or charging a battery creates heat. If the heat is generated faster than it is dissipated, the battery temperature increases and may cause the battery to experience a thermal runaway, i.e., uncontrolled self-heating due to exothermic chemical reactions. Even if a thermal runaway does not occur, a local hot spot may cause irreversible damage in cell components, thereby accelerating the decline of battery capacity. Much of the modelling work has been taking place within the automotive industries for development purposes and little has been spread to other application areas and end users.

It is only recently that large batteries have been introduced to other application areas. Maritime applications were the first sector to follow and were early in setting up requirements for thermal runaway propagation. It is also only recently that storage was introduced for stationary application at scale thereby calling for risk assessments for these types of applications.

2 Literature Review

The modelling of batteries, packs of batteries or battery modules is most often performed for evaluating factors under normal working conditions such as life-time performance (temperature, charge status, mechanical, pressure), however recently safety issues and abuse test modelling have become more and more important due to the increased use of Li-ion batteries in consumer applications, and as the number of fires and accidents that have occurred grows (Wang, Mao, Stoliarov, & Sun, 2019), (Wang, et al., 2012). Safety modelling of batteries includes but is not restricted to predicting the thermal runaway of a battery (Zavalis, 2013), the propagation of thermal runaways (Larsson, Andersson, Andersson, & Mellander, 2016) and emission of toxic gases from the event (Willstrand, Bisschop, Blomqvist, Temple, & Anderson, 2020). Modelling a thermal runaway is possible by utilising a thermal abuse model that can describe the evolution of heat transfer within the battery at elevated temperatures, this model can then be simplified to determine the heat diffusion in the battery pack and thus predict the spreading of a thermal event (Anderson, Sjöström, Andersson, Amon, & Albrektsson, 2014). This is done by computing heat transport in the battery pack by solving the heat diffusion equation numerically, where boundary conditions have to be estimated either by tabular coefficients or determined by simulation the surroundings using a conjugate heat transfer model. These models are often approximated as finite element (FE) or finite volume (FV) models. Simulating the spread of toxic elements from a thermal runaway event where the cell vents emit gas which is transported by flows either caused by the thermal event or ventilation utilises computational fluid model (CFD) where the pressure and velocities of the transported gases are solved in control volumes using Finite Volume Method (FVM). The simulation result is the tenability and may be used in a risk assessment (Willstrand, Bisschop, Blomqvist, Temple, & Anderson, 2020).

While modelling a thermal runaway presents insights into predicting the spread of a thermal event, the event itself may be predicted by short circuit models. Internal short circuit in cells and external mechanical stresses like nail penetrations, et cetera, have been explored for various cell types and battery packs. With hundreds of different types of cells, it is impossible to find experimental data on external short circuits for most of them which makes simulations of these scenarios valuable and necessary for different safety assessments.

Different commercial and open-source tools have been used to simulate battery thermal runaway event in previous studies. For example, the Ansys LS-Dyna was used to study the effect of mechanical abuse i.e., nail penetration, on the battery thermal event by coupling mechanical, electrical, and thermal process (Zhang, Santhanagopalan, Sprague, & Pesaran, 2015), (Zhao, Liu, & Gu, 2016). Comsol Multiphysics is a commonly used simulation tool for studying thermal propagation in battery modules by different researchers (Feng, Lu, Ouyang, Li, & He, 2016), (Ren, et al., 2017), (Ren, et al., 2018) (Abada, et al., 2018). GT-SUITE, a multi-scale, multiphysics software platform developed by Gamma Technologies was used to simulate battery pack thermal runaway for aircraft application (Harrison, Charles, Zenker, & Frank, 2019). The different software packages have different capabilities and studies on the applicability of each on different scenarios and comparisons with experimental data is lacking in the literature. In addition the studies are, in general, not applied to domestic situations. While failure such as nail penetration is unlikely in an end use situation, a short circuit might very well happen, both internal short circuits induced by a failure in the cell but also a short circuit from equipment external of the battery. The work presented here involves modelling of internal and external short circuits and the consequent thermal runaway in a battery assumed to be installed in a domestic environment. The work is conducted using GT-SUITE and the modelling also includes a review of the suitability of using GT-SUITE to study the spread of the toxic gases released by batteries.

GT-SUITE is a software platform including libraries for simulating fluid flow, all types of heat transfer, chemical kinetics, kinematics, and multi-body dynamics. It also has built-in quasi-3D¹ CFD and 3D FE solvers. GT-SUITE can import solid models from CAD to create 1D and 3D models and performs embedded 3D CFD and 3D FE thermal/structural modelling with all boundary conditions provided by the simulated surrounding complete system.

2.1 Thermal Runaway

Thermal runaway means the exothermic reactions in the battery is out of control, producing heat very rapidly, which in turn leads to a fast release of aerosol droplets from the electrolyte, which is flammable, and toxic gases with the increase of temperature and pressure inside the battery. A lithium-ion battery is only stable within a certain operational window, if it is put in a state outside of that window a thermal runaway can occur. A thermal runaway can be started by (i) thermal abuse, e.g., oven or fire heating, (ii) electrical abuse, e.g., overcharge or external short circuit, (iii) mechanical abuse, e.g., nail penetration or crash, and (iv) internal short circuit.

Thermal runaway mechanisms can be studied by performing tests in ovens and in Accelerating Rate Calorimeters. The test data can generate reaction kinetic parameters for a series of thermal decomposition reactions including: (i) the decomposition of the solid electrolyte interphase (SEI) layer, (ii) reactions between the anode material and electrolyte, (iii) reactions between the cathode and electrolyte, (iv) decomposition of electrolyte and (v) reactions between anode and the binder. The most used thermal decomposition reactions were proposed by (Hatchard, 2001).

A substantial amount of work has been published during the recent years regarding battery thermal behaviour using different multi-physics tools (García, Monsalve-Serrano, Sari, & Martínez-Boggio, 2022). The challenge is that most of the work focus on the thermal propagation behaviour of cell and module level. Little work focuses on the battery pack and system level, which is valuable due to the extremely high cost of tests when multiple factors will be tested. A well-validated and well-calibrated multiphysics model of battery thermal propagation can play an important role in designing safer batteries.

¹ GT-Suite simplifies a 3D space into a network of 1D pipes. It then solves 1D Navier-Stokes equations, namely the conservation of continuity, momentum and energy equations for this pipe network.

2.2 Short Circuits

An external short circuit is said to have occurred when the cell or the battery discharges via the external contacts but through a very small resistance such that the currents drawn from the cells are much higher than the safe levels of discharge. External short circuits result in an increase of cell temperatures to unsafe levels and might also be the cause for a thermal runaway. Different cells react differently to external shorts and the short characteristics depend on the cell type, cell chemistry, state of charge, ambient temperature, et cetera.

External short circuits in battery packs have not been studied as much (Kriston, et al., 2017) as other mechanisms that may lead to breakdowns such as overcharging or over discharging of batteries and internal short circuits in cells. Various experiments have been conducted on a cell level to study the effects of external short circuits based on different chemistries, different battery capacities (Conte, Gollob, & Lacher, 2009), different external resistances (Larsson & Mellander, 2014), et cetera, and can act as appropriate data for validation of the model. Simplified numerical simulations (Abada, et al., 2016), (Smith, Kim, Darcy, & Pesaran, 2010) and multiphysics models (Zavalis, Behm, & Lindbergh, 2012) are also available, but focus on a cell rather than a battery pack. Electrical models developed with inputs from experiments can be extrapolated to larger battery packs to predict changes in thermal and electrical parameters under an external short circuit condition.

2.3 Tenability Conditions

Tenable conditions can be defined as conditions which can be 'tolerated and endured', and the tenability limits are the point at which conditions are no longer able to be endured. Any limit is of course dependant on the context being considered and even within the bounds of "life safety of humans in fire events" can range from temperature limits (e.g. temperatures of 120°C in dry atmospheres will cause pain to any exposed skin or if breathed in (International Organization for Standardization, 2012)) to gaseous concentrations. When considering exposure to gaseous species the tenability limits will vary significantly depending on the gases present, are they asphyxiants (which prevent oxygen being captured by the lungs) or irritants (which cause damage via chemical burns or similar), are there gases which will work in conjunction with each other or is it a single species which to which there is exposure. For example, if it is an area where there may be a leak of carbon monoxide, but no other gases are expected to be present then a simple limit of 2000 ppm, as specified in Boverket's BBRAD code (Boverket, 2011), would be a suitable limit to consider. However, where multiple gases are present they may work in conjunction with each other to reduce tenability and more complicated measures such as the Fractional Effective Dose and Fractional Effective Concentration (for asphyxiants and irritants respectively) as defined in ISO 13571:2012 (International Organization for Standardization, 2012) may be more suitable.

It has been well established that Li-ion batteries produce flammable and toxic gases when they go into thermal runaway (Jie Sun, et al., 2016) (Andersson, Blomqvist, Loren, & Larsson, 2013) (Nedjalkov, et al., 2016) (Gager & Gary, 2017). The exact

make-up of the released gases is heavily dependent on the precise battery chemistry but will typically include CO, $CO_2 H_2$ and acidic compounds such as HF. To establish the risk that the release of these gases may pose to people, i.e. the risk of tenability limits being surpassed, the way they spread around a space and the concentrations that develop must be established. An increasingly common method of attempting to gain this understanding is via the use of standalone CFD simulations (Willstrand, Bisschop, Blomqvist, Temple, & Anderson, 2020) (Meraner, Tian Li, & Sanfeliu Meliá, 2021) with gas injection based on experiments (often with significant assumptions to expand from small to larger scale or transfer from one context to another) or with nominal values. The reliance on experimental data can make the studying of sensitivities within the design and of feedback loops difficult to accomplish in modelling. It is in these areas where coupling of the CFD analysis with electrical, chemical, and thermal models of thermal runaway within multi-physics software could give significant benefits to researchers and designers.

2.4 Available Test Data

The thermal runaway experiments were performed at RISE in 2019 (Bisschop, Willstrand, & Rosengren, 2020). The tested battery pack consisted of two live battery modules and six dummy modules. One live battery module contained 12 prismatic cells with anode and cathode material being C/NMC, nominal voltage being 3.7 V, and rated capacity being 28 Ah, respectively. Sand was filled in the dummy battery module and sealed. The case of dummy module was made of stainless steel. A circular opening of 24 mm in diameter on the body of the battery pack was made to expose a battery cell directly to a gas burner. This test setup aimed at simulating thermal propagation in case of a fire. Temperature was measured at different locations in the battery pack and the tests were recorded using a video camera.

For an electrical equivalent model, to simulate external short circuits, maps of temperature dependent state of charge vs. the open circuit voltage of the cell are necessary along with the temperature dependent state of charge vs. the internal resistance. In the above-mentioned tests, these parameters were not measured and are also not available in literature. Hence, data from (Wang, Bao, & Shi, 2017), (Bisschop, Willstrand, & Rosengren, 2020) is borrowed as a representative substitute. The capacity and the dimensions for calculating the surface area are taken from the datasheet of the considered cell. To validate the model and its behaviour, external short circuits are simulated and the temperature-time, open circuit voltage-time, state of charge-time and current-time plots are compared to literature.

3 GT-Suite

GT-Suite is a commercial simulation tool released by Gamma Technologies. It includes a multi-physics library for constructing multi-physics models including (i) mechanical, (ii) thermal, (iii) fluid, (iv) electric, (v) chemistry, and (vi) integrated systems (see Figure 1).



Figure 1 GT-Suite software package includes a multi-physics library.

As far as battery simulation is concerned using GT-Suite, the model can include three levels of physics as follows (see Figure 2):

- Level 1: 3-Dimensional (3-D) Finite element (FE) heat transfer simulations. Conjugate heat transfer simulation for studying the combination of heat transfer in fluid and solid, e.g., battery cooling.
- Level 2: 3-D FE model with battery electrical model by considering electrical equivalent in batteries
- Level 3: 3-D FE model with electrical chemical model for considering battery ageing, change of cell performance and resistance. Note that the thermal runaway reactions are available in the AutoLion package.

The computational cost increases with the increase of more physics in the model. It is worth noting that an extra license of GT-AutoLion is required.



Figure 2 Battery models in GT-Suite

The procedure for setting up the model includes the following steps:

- 1. Construction of CAD geometry in GT-SpaceClaim
- 2. Discretization of the solid and fluid domain in GEM3D
- 3. Set up the model by connecting different parts, applying proper initial and boundary conditions in GT-ISE.
- 4. Run the simulation in GT-ISE
- 5. Post-processing the results in GT-POST.

To summarize, GT-Suite is a multi-physics software which has great potential to be applied in battery safety designs. The advantages of the program are:

- Diverse Multi-physics libraries, models available including thermal finite element model, electrical model, electrical-chemical model, flow, heat transfer, radiation and so on.
- Low computational cost
- The model is scalable (simulate problems in large-scale, e.g., battery pack, energy storage system)
- Tools available for analysing big data, e.g., neural networks, metamodel (different mathematical models which can be trained by many multi-physics simulations to produce fast results).
- Technical support from application engineers by the vender.

The disadvantages of the programs are:

- License cost.
- Extra cost associated with GT-AutoLion if thermal runaway reactions will be studied.
- More licenses are needed for running simulations in parallel.

4 Thermal runaway modelling

As part of this project a battery thermal runaway model containing 12 prismatic cells based on 3-D FE approach was built using a GT-Suite multi-physics software. The computed thermal runaway time instants versus thermal runaway cell number were compared with full-scale experimental data with reasonable agreement. A quantitative sensitivity study on the model input parameters and model space and time resolutions on the computed start time instant and time duration of thermal runaway was also performed. On the basis of this work the multi-physics model for battery thermal runaway process is promising and worth to be applied with care for designing safer batteries in combination with full-scale testing. More detailed information about the results of the study is provided in a manuscript (Huang, C.; Bisschop, R.; Anderson, J., 2022).

5 Short Circuit Modelling

5.1 Introduction

External short circuits in cells are when the terminals of the cells are in contact with each other with a very small resistance externally. The extremely small resistance causes a large amount of current to pass through the cell which because of the internal resistance of the cell increases the cell temperature drastically. This may or may not be drastic enough for a thermal runaway to be initiated. The initiation of a thermal runaway depends on various external and internal factors. The external short circuit resistance, the initial state of charge, the initial operating temperature, common conductivity as a result of ventilation, etc decide if the cell goes into a thermal runaway after an external short. The cell chemistry also plays a major role in deciding if a thermal runaway will take place. The release of gases, build-up of pressure, etc are a direct result of the chemical composition of the electrolyte. For the sake of simplicity only an electrical equivalent model of a cell is considered in this project and not an electrochemical model instead.

The objective is to assess if GT suite is suitable for modelling of external short circuits in lithium-ion modules or battery packs. This said, the short circuit model goes hand in hand with the thermal propagation model. A single module consisting of 12 cells is modelled and the simulations are run in three configurations; single cell series module, 4 cell series module and 12 cells series module. To simulate an external short circuit, an external resistance with a very small value is used to connect the two terminals of the module. The output of the model, which is primarily the temperature versus time plot, is compared to the experimental data from different short circuit tests conducted. It is also used as an input to the thermal model to initiate the thermal runaway condition.

5.2 Data and References

As inputs to the electrical equivalent model, a map of temperature dependant open circuit voltage versus state of charge and temperature dependant internal resistance versus state of charge for the cell used in the model are required. Other input parameters required are the capacity of the cell, which is available from the supplier datasheet, and the physical dimensions of the cell from which the area for heat transfer is calculated. For this model, prismatic cells with a capacity of 28Ah each have been used. While the capacity and the physical dimensions of this cell are available, the temperature dependant open circuit voltage and internal resistance versus the state of charge values are not available. As an approximation, these two maps have been borrowed from literature (Wang, Bao, & Shi, 2017) and are values measured for an 18650 cell. A more representative model would rely on data collected experimentally on the same 28Ah cells.

To validate the output of the model, the temperature versus time and the voltage drop versus time is compared with experimental data. Only the trends can be compared as actual experimental data is not available for these cells. Also, validating results for a module is harder as experimental data is only available on a single cell level and extrapolating it to a module might not be a linear exercise.

5.3 Model setup

The objective is to have 12 cells connected in different configurations that drain through a fixed external resistance. The currents in the system due to the value of the external resistance together with the resistances of the electrical connections are computed and used to calculate the change in temperature. These values are also to be used as input values to the thermal model. In case of a thermal runaway, which essentially is a threshold value for temperature, the thermal model takes over. GT-Suite allows lumping of cells to have 1 battery pack element instead off multiple cells connected in a certain configuration. However, in this model individual cells are used as elements as simulations are run over different configurations of the cells. The capacity of each cell is defined as a constant based on the datasheet value, which in this case is 28Ah. The initial SoC is defined as a variable parameter so that it can be easily



Figure 3(a) schematic of a cell, bus bars and the connection to the external resistance. (b) shows a snippet from GT-Suite shows the connection of the bus bars to the cell and the connection of the cell to the thermal model. (c) schematic of 4S3P module, one of the three configurations modelled.

varied in the case set up before every run. The load type for every cell is set to be dependent on the external electrical connections and not by a current or power request. This ensures that the current is a computed value based on the external resistance and not a constant which has been pre-defined. Circuit parameters including open circuit voltage and internal resistance for both charge and discharge cycles are defined, see Figure 3. These are temperature dependent values and are borrowed from literature as mentioned in section 4.2.

"Internal thermal node with external thermal connections" option allows the linking of the cell to the casing and jelly roll elements of the thermal model. The internal thermal node object and the area of heat transfer are defined as parameters. Approximate values of thermal properties are used, and the conductivity is set as 3 W/(m-K), density as 100 kg/m³ and specific heat as 1100 J/(kg-K).

In the first configuration, all 12 cells are in parallel to each other implying the module voltage to be the same as a single cell voltage of 3.7 V. In the second, 4 cells are in series and three strings in parallel to each other bringing up the module voltage to 14.8V as in Figure 3(c). The third configuration has 6 cells in series and two strings in parallel with a module voltage of 22.2V.

5.4 Results and Discussion

With the electrical model acting as the input to the thermal model, the most interesting output of the simulation is the change in temperature of the cells with respect to time. From an electrical standpoint, given an external short circuit scenario the temperature increase is dependent on the current that flows through the cells. This current is determined by the value of the external resistance through which the short takes place and the voltage level of the battery pack. 12V and 24V systems are widely used battery levels and hence the four cell and six cell series modules have been modelled. For comparison a single cell series module is also modelled.

The output of the model follows the trend of increase in temperature of the cells when subjected to a short circuit that is noted in literature. However, it is only the trend and not the actual values or the actual rates of increase that can be compared to experimental results. This inaccuracy can be attributed to the lack of a more sophisticated and detailed model consisting of electrochemical equations specific to the cell as governing factors. Also, as previously mentioned the internal resistance map and the open circuit voltage map used are that of a generic 18650 cell and not the pouch cell whose other parameters have been used in the model.

While as a trigger the model works, several inconsistencies are to be noted, some of which might have been a result of the limited time frame of this project. Firstly, the rate of increase in temperature is not a reflection of experimental outcomes. The time taken to reach the threshold temperature to initiate the TR is much longer than what it would take in reality. As comparison of these results are difficult due to lack of experimental data on short circuits in entire modules, simulation results on a single cell can be compared to experimental outcomes. Secondly, the values of current, cell voltage and state of charge do not behave as they would in practice. The current in the simulation reaches a stable nonzero value and so does the cell voltage. This would be very different in reality as the voltage would steadily drop to a near zero value upon an external short circuit and the current would initially jump to a very high value but would plateau and then steeply reduce to zero as well. Upon disconnection, depending on the scenario, the open circuit voltage may go up a little bit but not to operational levels. However, in the simulations, irrespective of the configuration, the current and the voltage become a constant after a certain period. On the other hand, the state of charge steadily drops and continues to decrease in the negative Y axis indicating a negative SoC which is meaningless. This means that despite a TR, there is a constant current flowing through the cells that further contribute to the heat generated. Even when a higher resistance is used as a load, the temperature increase never stops as the current never stops flowing which would mean that the energy in the cell is never fully depleted. Figure 4 shows a comparison of plots of changing open circuit voltage and currents between experimental values and the simulated values. Despite time being on a linear scale for the simulated values, the curves are not as steep as expectations.



Figure 4(a) Experimental setup from (Kriston, et al., 2017). showing a 10Ah pouch cell subjected to an external short circuit through a $10m\Omega$ resistor. (d) Drop in measured current and voltage. (b)(c) Stabilization of voltage and currents at an arbitrary value from the simulation and (e) SoC decreasing to negative values in the simulation.



Figure 5 Comparison of change in temperature between the three different battery configurations. Higher terminal voltage means more current and a faster rate of increase to reach the threshold level. In case of 1S12P, the terminal voltage is the least at 3.7V and correspondingly a slower rate of increase in temperature is noted. In case of 4S3P with a terminal voltage of 14.8V, the threshold is reached in half the time as compared to the first case. With the 6S2P configuration and a 22.2V, although the voltage is almost twice, the threshold is only reached marginally faster than the 14.8V module.

Figure 5 shows the comparison of the temperature versus time plots for the three different battery configurations. With higher terminal voltages and the constant external resistance higher currents are drawn from the cells as expected. Higher currents imply higher temperatures and quicker rates of increase. This can be observed

from the simulations. However, the difference in the times taken for the increase in temperature do not reflect theoretical expectations. Fundamentally, for a given amount of energy dissipated because of a current through a resistance, the time taken is inversely proportional to the square of the current. This implies that increase in the current by a factor of two should shorten the time it takes to dissipate a given amount of energy by a factor of four. With the increase in currents between the 4S3P module and the 6S2P module, this expected decrease in time it takes to reach the TR threshold is not seen in the simulated results.

5.5 Conclusions

Simulations of short circuits as such are becoming more relevant with the exponential increase in the use of lithium-ion batteries across applications. The use of GT-Suite to conduct such simulations have been attempted and the results have been discussed as above. Considering those, the following conclusions and suggestions can be considered.

- On a more fundamental perspective, comparison of the experimental data to the outputs of the simulation is not entirely accurate as the input parameters to the electrical model is from different cells and references. As a result, it can be very useful to conduct tests on one particular cell that would be modelled, and all parameters be used from those experiments.
- Electro chemical equations should be added to the models to make them independent of measured internal resistance values. GT-Suite offers many nuances for modelling and requires significant time to learn and explore optimal methods depending on requirements.
- The obtained results from the above simulations can only be used as a starting point and not as absolute values for neither triggering the thermal model nor for accurately simulating a battery under an electrical load.
- GT-Suite seems to be a promising software to model external short circuits in cells and battery packs. However, exploring all possible tools and intricacies will take significant time.

6 Tenability Conditions Modelling

6.1 Introduction

The potential benefits to having coupled Multiphysics simulations are significant, particularly for automation of cases studying the influence of variables across different the modelled aspects or for modelling feedback loops (e.g. gas releases setting off a detector which activates a cooling system and then monitoring any impact on propagation via a thermal model). However, coupling of the computational fluid dynamics (CFD) portion of GT-Suite's toolbox with the electrical and thermal models discussed earlier is possible, but adds an additional layer of complication. Prior to attempting this it should be assessed if the simplifications inherent in GT-Suite's 1D CFD is appropriate for assessing tenability conditions within a space. A simple comparative analysis against an alternative CFD tool has been undertaken to provide a

first step. The case considered will track the spread of a single gaseous species released into a room size compartment and the comparison will be made against a matching simulation carried out in Fire Dynamics Simulator (FDS). Note that neither FDS or GT-Suite have been validated (indeed there is limited readily available validation case data to be used) for the simulation of diffusion of gaseous species in a 3D space and it is possible neither give fully accurate results. However, FDS uses a 3D CFD model as opposed to GT-Suites 1D pipe approximation (flow driven by pressure differentials and turbulence not solved for, may also not include buoyancy although this is unclear from the software UI and guides reviewed) so should provide a more accurate representation and been used for this sort of modelling in the past (Willstrand, Bisschop, Blomqvist, Temple, & Anderson, 2020), (Meraner, Tian Li, & Sanfeliu Meliá, 2021).

6.2 Model Setup

6.2.1 Case Overview

The modelled case represents a 3 m x 3 m x 2 m (depth x width x height) room with natural ventilation provided by a low level inlet and high level outlet on opposite walls. An obstruction, measuring 30 cm x 70 cm x 35 cm (depth x width x height), representing the casing of a battery back is placed in the centre of the room. The 'exhaust' gas that is to be tracked is inserted into the model via a vent located at the middle of the upper surface of the battery pack. A sketch of this geometry can be seen in Figure below.

The gas used to represent "battery release gas" in the models was HCN with a peak release rate of 10 g/s at a temperature of 40° C. The release rate ramps linearly from 0 g/s at the initiation of the model to a peak at 600 s before ramping back to 0 at 1200 s, see Figure 7. The models were run for 1200 s and measurements of gas concentrations are to be taken for comparison at 9 locations listed in Table 1.

As a comparative study of the CFD capabilities is being conducted only and no secondary analysis (i.e. actual tenability conditions) are conducted the specific gas or gases injected into the space is not key to the results. The gas used in both models must simply be the same. HCN was selected as it is not a component of air and there is a built-in specification for it in both FDS and GT-Suite. Additionally, a small amount of HCN is also released from some batteries (Willstrand, Bisschop, Blomqvist, Temple, & Anderson, 2020) and so can be considered partially representative of gases released in thermal runaway. The release rates and timings are simple arbitrary values chosen for the basis of this comparative study only and are not representative of any particular battery.



Figure 6. Sketch of the simple room geometry used for CFD comparison models.



Figure 7. Arbitrary HCN release rate representing "battery gas" for the purposes of the comparative model.

Table 1. Gas concentration measurement location

Location	X co-ordinate*	Y co-ordinate*	Z co-ordinate*
Number	(m)	(m)	(m)
1	0	0	1
2	0	0	1.2
3	0	0	1.4
4	0	-0.4	1

Location	X co-ordinate*	Y co-ordinate*	Z co-ordinate*	
Number	(m)	(m)	(m)	
5	0	-0.4	1.2	
6	0	-0.4	1.4	
7	0	0.4	1	
8	0	0.4	1.2	
9	0	0.4	1.4	
* The origin of the compartment is at the centre of the plan at				
floor level.				

6.2.2 GT-Suite Model

The geometry of the model, e.g. flow volume, vent locations and ambient conditions, were set up in the GEM3D element of GT-Suite's pre-processors. The flow volume itself is created rather than the full domain with obstructions. The vents to outside and for the flow are modelled as short pipes starting outside of the flow volume and finishing inside. These are modelled with square cross sections with 200 mm sides.



Figure 8. Basic geometry visualisation and setup from GEM3D.

The flow volume is sub-divided into 200 mm long pipes for use in the CFD analysis and inserted as a sub-model within the main model, see Figure 8. The 200 mm subdivision of the flow volume was the maximum subdivision that the hardware (a 2018 Lenovo ThinkPad laptop with an i7-8550U CPU and 16 GB of RAM) was able to manage without crashing. Further subdivision may be possible with more powerful hardware, but may cause other usability issues, see section 6.4. Within the main model the definitions for the inlet and outlet vents are set (20°C and atmospheric pressure) as

well as the "battery gas" flow, Figure 9. The HCN is specified as the inbuilt "hcn-NASA" fluid within GT-Suite.



Figure 3. Main model setup in GT-Suite showing flow volume Sub-Assembly, the HCN input flow (BoundaryFlow Species-1) and ambient vents.

Monitoring of HCN concentration at the locations noted in Table 1 are set within the sub model.

6.2.3 FDS Model

Two versions of the scenario were modelled utilising FDS with varying mesh sizes. Both had cubic cells and they had cell dimensions of 20 cm, to match the subdivision of the GT suite model, and 10 cm mesh to allow for FDS mesh sensitivity. A representation of the geometry as modelled in FDS can be seen in Figure 0. The HCN used was the built in "Hydrogen Cyanide" species in FDS.



Figure 40. FDS model as visualised in Pyrosim (an FDS pre and post processor). Note the walls closest the camera and ceiling are rendered as wireframes.

6.2.4 Results

The concentrations of HCN at each of the measuring locations for the GT-Suite, FDS 20 cm mesh and FDS 10 cm mesh models are shown in Figure 11, 12 and 13, below. The results are show a notable difference in recorded concentrations between the two models, with the GT-suite model results giving pure HCN in the locations directly above the gas inlet, while the other locations reached concentrations between 10% and 27% (100,000 to 270,000 ppm). In the FDS models the magnitude of the concentration directly above the inlet reached a maximum of 35% (350,000 ppm) at location 1 and showed a greater variation with height as the concentration at location 3 peaked at approximately 27%. The other 6 locations were grouped closer together than in the GT-Suite model all reaching maximums of around 20%. Both FDS models give similar results to each other with the main difference being the level of noise in the results, with the larger 20 cm mesh having less noisy results.



Figure 51. HCN concentrations measured in the GT-Suite model plotted against time.



Figure 62. HCN Concentrations as measured in the 10 cm mesh FDS model.



Figure 73. HCN Concentrations as measured in the 20 cm mesh FDS model.

6.3 GT-Suite Usability

In comparison to setting up the scenario discussed in this section in FDS (or a FDS preprocessor such as Pyrosim) there were a few differences in the processes.

GT-suite uses a node-based representation of the models, see Figure 3 above and Figure 8. Where there is a simple model with a small number of nodes, such as the main model for this study, this can make it very easy to see at a glance the structure of the model and what is being represented. However, in some instances it can also be very unclear and difficult to manage. This is the case with sub model of the flow volume of this study, Figure 14, where the large number of nodes (representing joints in the simplified 1D representation utilised by GT-suite), often on top or very close proximity to each other, makes reading and navigating the model significantly more difficult.



Figure 84. Screenshot of the flow volume sub model from the GTISE model pre-processor.

The method for logging results is also unusual when compared to several other CFD software suites. In FDS for example, the data that the users wishes to have logged and reported is specified independently of the definition of the models calculation elements. This will include the location specified as co-ordinates, in the case of point measurements, or bounds, in the case of area measurements, along with the data type (temperature, species concentration, etc.). In GT-Suite the data to be tracked is defined by reference to the node at which it is calculated and not via an independent location definition. For example, in the model within this study the location for each point where the HCN concentration was to be measured was specified in reference to the node defining the 1D flow junction closest to that location (e.g. "compartment_3_4_4"). In smaller models or in models of specifically designed systems where the geometric location is of limited importance and what is vital is where along the system it is, this method can have a significant advantage, however where you have a situation with a large volume and the geometric location is important this becomes significantly harder to manage. This is further complicated by the fact that the individual flow nodes and connections are autogenerated by GT-Suite upon export of the geometry from GEM and the individual nodes do not include any location data

(simply what distance away the other nodes they are connected to are). This means that there is no simple way, that we could find, of establishing which nodes are representative of the correct geometric location. To overcome this, 'sensors' were defined within the GEM3D file (note that 'sensors' in GT-Suite are for providing a control input into another part of the model, e.g. activating something when a certain temperature limit is met, and cannot be used just to log data) prior to export for setting up the CFD model. When the flow volume model is then opened in the primary model pre-processor, these sensors are attached to the appropriate nodes and the names of the correct nodes can be identified for setting up the data logging. After this the sensors need to be deleted prior to running the model (otherwise the model will crash). This provided a means for the model discussed within this section of the report to be set up but required significant additional time beyond what would be expected for the model's complexity and is a method that would not scale if a large number of locations are needed to be reviewed.

6.4 GT-Suite Tenability Assessment Suitability

The large variation in results between the GT-Suite and FDS models indicates that GT-Suite is not suitable for assessing tenability conditions within a space. The variation in results (~pure HCN directly above the opening, with lower levels elsewhere) is likely due to the 1D pipe approximation that GT-Suite uses for the flow simulation. In a 1D pipe the assumption is of laminar flow and at junctions this will favour flow straight across any junction in the direction of the flow, with less flow directed in any other directions, see Figure 15. In comparison FDS models the turbulent flow expected in large spaces and will subsequently result in a wider dispersion of released gases.





In addition to the concerns regarding the accuracy of the results in this context there are usability issues, as described in section 6.2.2, that limit the practicality for setting up models in larger spaces.

Where GT-Suite would have a place in simulation-based studies of tenability conditions after thermal runaway is in assisting developing the gas release rate input curves for CFD analysis in other software. Thermal runaway and propagation models as discussed in other sections of this report could be used in conjunction with, either chemical models or single cell gas release experimental data, to develop time histories of gas release for input into CFD models conducted elsewhere.

7 Discussion and Conclusions

As the lithium-ion batteries continue to increase in capacity and become increasingly common in our lives the risks associated with them and therefore the importance of understanding their behaviour grows. More research needs to be done to ensure a safe transition towards electrification with massive use of Lithium-ion batteries. Multiphysics suites, such as GT-Suite can have an important role in carrying out and supporting this research, particularly, as demonstrated in the studies described in this report, in investigations regarding the electro and thermal responses surrounding thermal runaway. While the simplified CFD model in GT-Suite is not suitable for assessing the tenability conditions within a space when a battery goes into thermal runaway, GT-Suite can however assist in these investigations as a method for developing appropriate gas release curves via simulation of the propagation of thermal runaway through a battery pack in combination with experimental data for gases released. A selection of additional studies which could take research forward in this area are described below:

- Develop thermal runaway reaction mechanism by performing Accelerating Rate Calorimeter (ARC) experiments and simulations.
- Improve understanding of battery thermal runaway process by incorporating (i) electrochemical model, (ii) thermal decomposition reaction kinetics, and (iii) thermal model.
- Battery thermal propagation simulations in larger scales, e.g., several battery modules in a battery rack, Battery Energy Storage System (BESS).
- Parametric studies of improved safety design of battery module and system, e.g., improved isolation between battery modules.
- Battery thermal runaway mitigation simulations, e.g., integrated fire extinguishment channels in the battery module and pack.
- Develop a well-calibrated, short-runtime battery thermal propagation model with the help of Machine Learning. Integrate the short-runtime model into Battery Management System (BMS) to make real-time decision of mitigation strategies.
- Comparison study between gas release predicted via simulated thermal runaway propagation and experimental test.

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