Thermal Runaway in Electric Vehicle Crash Simulation using LS-DYNA

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1 Introduction

Safety is an important functional requirement in the development of large-format, energy-dense, lithium-ion (Li-ion) batteries used in electrified vehicles. Many automakers have dealt with this issue by enclosing the batteries into robust protective cases to prevent any penetration and deformation during car crashes. While this worked well for first-generation vehicles, consumers are increasingly interested in higher range, which makes overengineered heavy protective cases detrimental for range. A more detailed understanding of battery cell behavior under abuse becomes is therefore necessary to properly make design trade-offs.

Computer -Aided Engineering (CAE) tools that predict the response of a Li-ion battery pack to various abusive conditions can support analysis during the design phase and reduce the need for physical testing. In particular, simulations of the multi-physics response of external or internal short circuits can lead to optimized system designs for automotive crash scenarios. The physics under such simulations is quite complex, through coupling structural, thermal, electrical, and electrochemical aspect. Moreover, it spans length scales with orders of magnitude differences between critical events such as internal shorts happening at the micron level, triggering catastrophic events like the thermal runaway of the full battery. The time scales also are quite different between the car crash happening in milliseconds and the discharge of the battery and temperature surge taking minutes to hours.

A distributed Randles circuit model in Ansys LS-DYNA can mimic the complex thermo-electric behavior happening in the electrodes and separators of lithium-ion batteries. The Randles circuit model is coupled with the mechanical solver of LS-DYNA where the deformations due to a battery crush allow the definition of criteria to initiate internal shorts. The internal shorts produce Joule heating which is transferred to the thermal solver of LS-DYNA where the temperature rise triggers exothermal reactions leading to thermal runaway.

In order to correlate mechanical deformations to the onset of internal shorting, subsequent appearance of thermal runaway, resulting gas emission, fire, and/or explosion, a series of crush experiments on automotive pouch cells and a multi-cell arrangement have been performed by Ansys. Benchmarks between experimental and numerical results from LS-DYNA allowed the identification of cell multiphysics properties. The cells were then used in different simulations of full electric vehicle crash. This paper will present the workflow from single cell experiments to full crash modeling including the sequence of steps, which can be repeated for other electric or hybrid vehicles with different battery cells.

2 Presentation of the model

The general process of a catastrophic thermal runaway due to a crash or a thermal abuse in a vehicle is described in Figure 1. A mechanical deformation of a cell due to the crash induces an internal short with joule heating that brings the cell to a temperature high enough for the exothermal reactions to start, which, in turn, increases the cell temperature to very high levels. This high temperature triggers swelling and venting of the cell and possibly ignition. This ignition can then propagate from cell to cell through thermal contact.

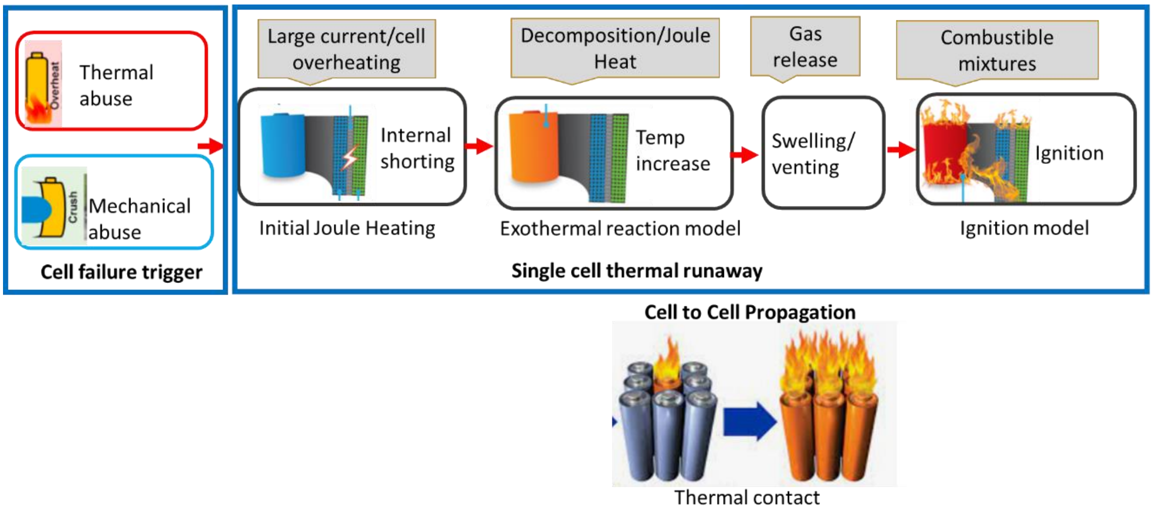


Fig.1: Different steps of a catastrophic thermal runaway in an EV or hybrid vehicle. Image adapted from Sinovoltaics

In order to simulate thermal runaway from cell to system within LS-DYNA, different models were developed for the different stages, and benchmarked against experimental results performed by Ansys on an automotive-grade pouch cell. This cell will be referred to as the “Ansys test cell” for the purposes of this paper.

Fig.2: Pouch cell used for the Ansys experiments (Ansys test cell)

The remainder of the paper describes the methods used for the different steps, the results of the benchmarks and walks a user through onsetting up the same model on other cells, module, pack, or battery type.

3 Cell Thermal Runaway Triggered by Mechanical/Thermal Abuse

The first stages of the process, i.e. going from the mechanical deformation of a cell due to a crash, or a localized thermal abuse to an internal short, joule heating and exothermal reaction is done by a coupling between the mechanical/EM/thermal solvers of LS-DYNA It has been described in detail in [1-7]

3.1 Setup of the Mechanical Parameters

`*MAT_CRUSHABLE_FOAM` (**`*MAT_063`**) is used to simulate the cell's mechanical properties. Different indenter shapes were used in the Ansys experimental tests including flat, cylindrical, and spherical. Quasi-static crushes as well as fast dynamical ones were performed. Figure 3 shows a benchmark between numerical and experimental results. Flat compression test data was used for material calibration to develop a homogenized cell through thickness stress-strain response. The material properties were then validated against other indentation load cases.

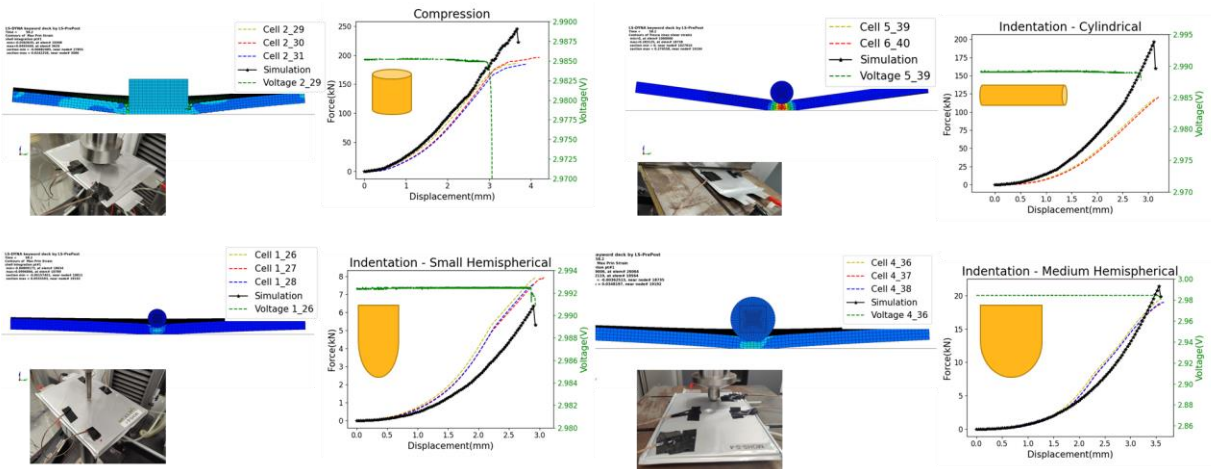


Fig.3: Benchmark between experimental and numerical data on quasi-static crush experiments with different indenter shapes.

3.2 Setup of the Randles Parameters

Cell’s internal short and initial joule heating are modelled using a distributed equivalent circuit approach, called Circuit Model [1]. In this study, the homogenized Batmac model [7] was used. These circuits have the advantage that they are computationally inexpensive compared to a full electrochemical model. The Batmac model reproduces the main features of a cell especially during the short time of a crash (where ageing effects are not relevant and are therefore not considered), it is easy to connect the cell to external circuits (connectors, buses, …). The main interest, though, is that it is easy to model external as well as internal shorts.

The Randles parameters of the Randles Circuits Model, which are used to represent the cell’s electrical properties, can be obtained from capacity test and Hybrid Pulse Power Characterization (HPPC) test on one cell, as described in details in [8].

Figure 4 shows the electrical components of the Randles Circuit Model and the contribution of each component to the cell voltage response as the cell gets charged and discharged. An example of the model prediction on the Ansys test cell’s voltage response under the HPPC tests is also shown.

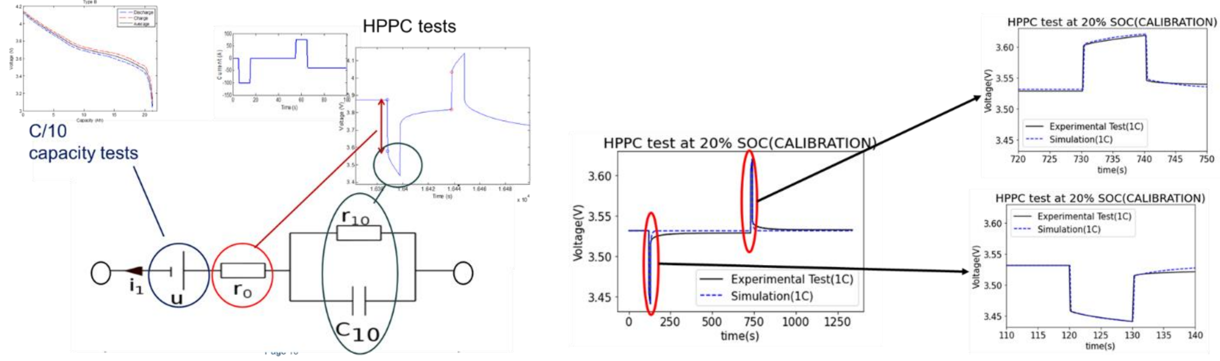
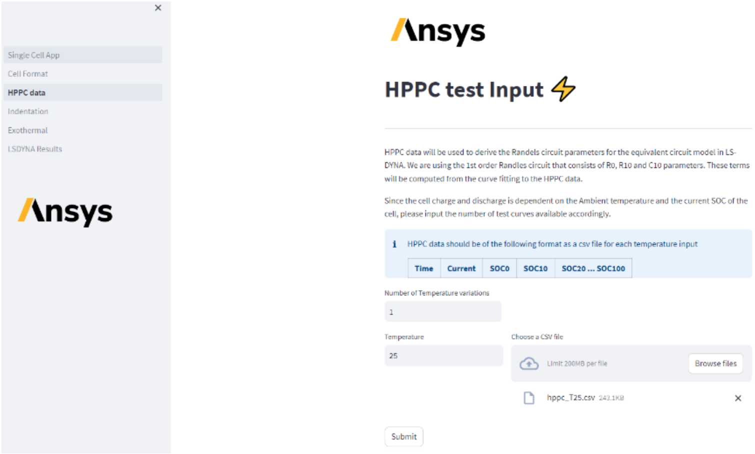


Fig.4: Setup of the Randles parameters given HPPC test results, with the comparison of the HPPC voltages between experiment and simulation on the Ansys test cell.

Considering that the HPPC test data is collected at several SOCs and the test is repeated at multiple temperatures, we felt a need to automate the process of extracting the Randles circuit parameters from the HPPC test data. Ansys has developed a workflow using pythonic APIs of several of its tools to fully automate the cell characterization process. The curve fitting required to extract the Randles parameters is built into this workflow. The image below shows the web interface that can be used to easily extract the Randles parameters from the test data. The extracted R0, R10 and C10 parameters are written out as **`*DEFINE_CURVE`** and **`*DEFINE_TABLE_2D`** so that it can be easily used in the input file for **`*EM_RANDLES_BATMAC`** models.



HPPC data will be used to derive the Randels circuit parameters for the equivalent circuit model in LS-DYNA. We are using the 1st order Randles circuit that consists of R0, R10 and C10 parameters. These terms will be computed from the curve fitting to the HPPC data.

Since the cell charge and discharge is dependent on the Ambient temperature and the current SOC of the cell, please input the number of test curves available accordingly.

HPPC data should be of the following format as a csv file for each temperature input

Time	Current	SOC0	SOC10	SOC20 .... SOC100

Number of Temperature variations: 1

Temperature: 25

Choose a CSV file: Limit 200MB per file

hppc_T25.csv 243.1KB

Fig.5: Web interface for the automated Cell Characterization App

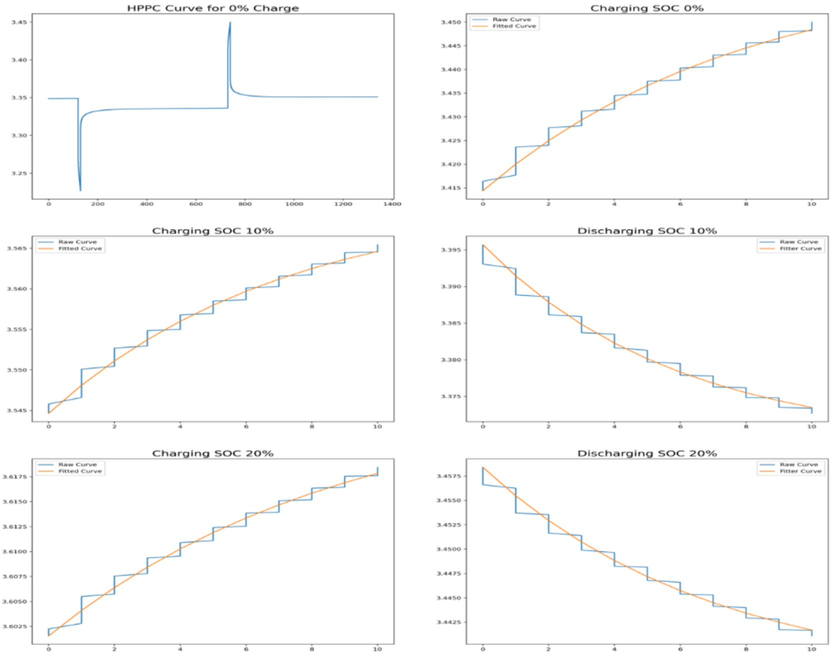


Fig.6: Sample Curve fit generated by the Cell Characterization App

3.3 Setup of the External Short

External shorts can be triggered using the **`*EM_CONTROL_CONTACT`** and **`*EM_CONTACT`** cards, where a path for the current will automatically be detected if 2 conductors come in contact, like in the tabs, buses, or other connector areas. The current flowing through these shorted paths can generate extra Joule heating, and hence temperature increase.

3.4 Setup of the Internal Short Parameters

The **`*EM_RANDLES_SHORT`** card allows the user to trigger a local internal short as a function of mechanical parameters such as strain or stress, or thermal parameters such as temperature (e.g., internal short induced as a result of separator melt). Parameter identification including mechanical/thermal threshold to induce internal shorts as well as short resistance are highly test data dependent. The short activation threshold can be identified based on failure strain/stress as simulated in the finite element model. To capture the voltage drop during the internal short event including magnitude and rate of change, sensitivity analysis on the amount of the short resistance was also performed. This calibration process provides a foundation for the cell running into internal shorts as a result of mechanical abuse. It is assumed similar voltage drop response would also occur in more complicated systems such as battery modules and battery packs.

Figure 7 shows the benchmark of the voltage drop during an internal short on the Ansys test cell under two different impactor profiles.

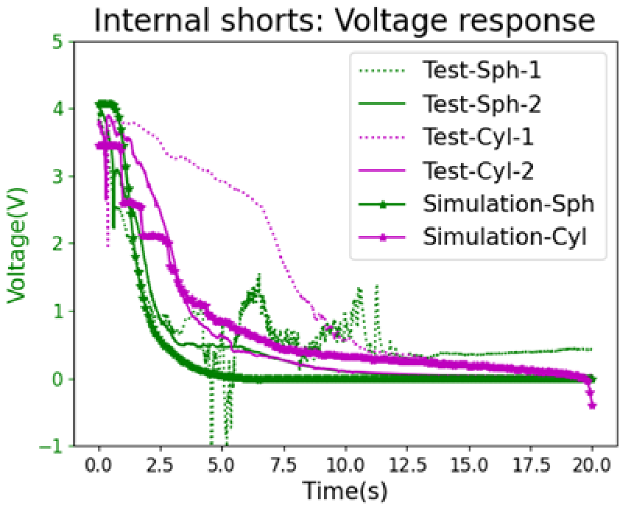


Fig.7: Benchmark between test results and numerical simulation showing the voltage drop after the onset of the internal short. The green lines correspond to a spherical indentation and the pink ones to a cylindrical indentation.

3.5 Exothermal Reaction Models

The NREL's 1 and 4 equations models [9] have been implemented in LS-DYNA, through the **`*LOAD_HEAT_EXOTHERMIC_REACTION`** card.

Another way to set up the exothermal reaction is through the **`*EM_RANDLES_EXOTHERMIC_REACTION`** card. Similar to the internal short, this card allows users to implement desired thermal runaway reaction model by adding a heat source to the cell model. The heat addition can be triggered via user-defined values such as temperature. The temperature difference between pre-thermal runaway and thermal runaway would inform users of the amount of heat/power that is required to simulate the temperature rise. The temperature drop after thermal runaway can be modeled using convection capability to release heat. This process calibrates the cell's capability to exhibit a thermal runaway event provided the temperature threshold is met. This card was used on Ansys test cell and the comparisons between experimental and numerical temperatures are given in Figure 8.

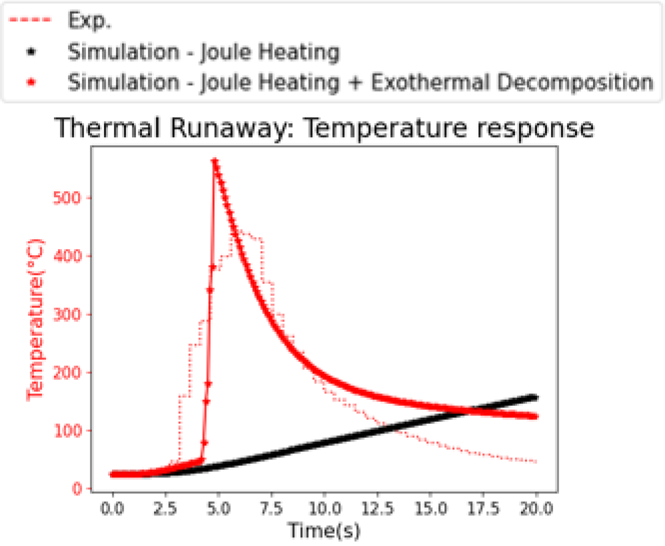


Fig.8: Benchmark of temperature rapid rise and slow drop caused by an internal short between experimental (light red), numerical results with only the joule heating due to the internal short (dotted black), and the numerical results with joule heating + exothermal reaction (dotted red).

4 Swelling and Venting

The next step of the process is gas generation within cells during the thermal runaway event. To simulate cell swelling and gas venting in LS-DYNA, we use the airbag particle method (**`*AIRBAG_PARTICLE`**) where the gas particles are generated and accumulated within the cell. The particle accumulation within the cell causes the cell to expand. Once a burst criterion is reached, the gas particles from the cell model are released to the vessel.

The required input to simulate the cell swelling and venting would be gas information including gas mass flow rate and gas temperature time history. The gas information is measured during the test in a pressure vessel and multiple temperature probes are located within the vessel to measure the gas temperature as the cell vents. The swelling force is also measured from the clamp plates where the cell sits in between. Figure 9 shows the experimental test setup

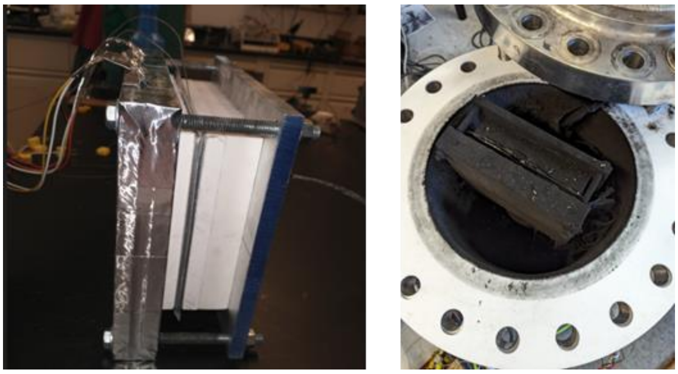


Fig.9: Experimental setup used to measure the gas emission of the cell during thermal runaway.

Figure 10 shows the benchmark between the experiment and simulation. The simulation captures the general trend of the experimental cell swelling force data. The temperature and the pressure data for the first 5 seconds are in good agreement with the model.

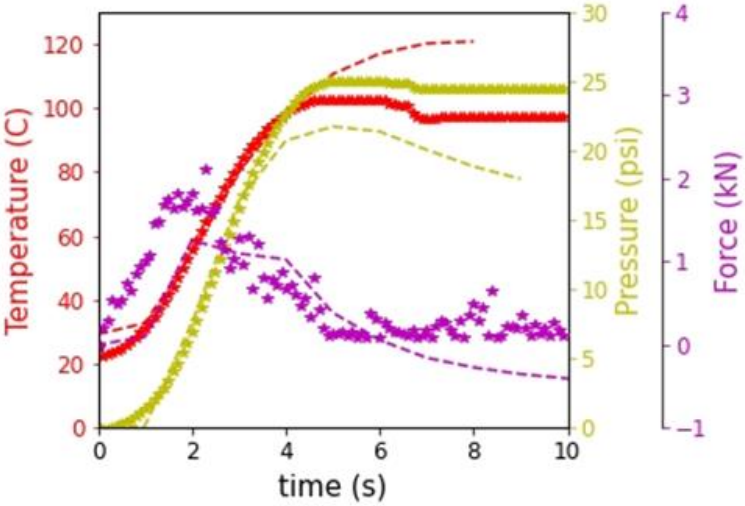


Fig.10: Experimental (dashed) vs numerical (dotted) gas pressure (yellow), force (purple), and temperature (red) vs time.

We are currently exploring other methods giving more accurate results on the gas flow profile. However, the current method already gives relatively good results on the integrated values, as shown on Figure 10.

5 Cell to Cell Propagation

In order to study the propagation of a thermal runaway from cell to cell, 5 cells were stacked up and a thermal runaway was triggered on the top cell through thermal abuse. The experiment was performed using the Ansys test cell and the simulation was done using the same methodology as previously mentioned. Figure 11 shows a comparison between the experimental and numerical temperatures on the 5 cells, with a very good agreement between the 2.

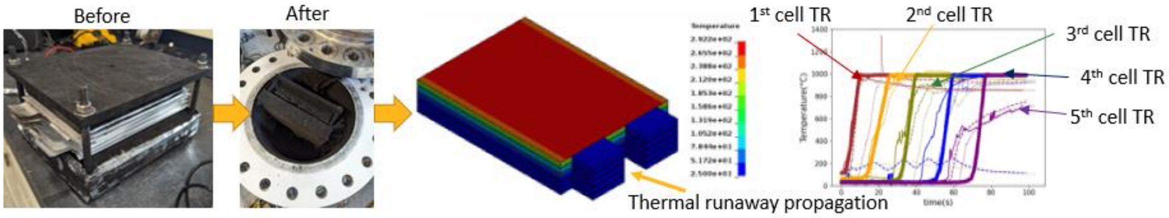


Fig.11: Propagation of the thermal runaway across a module of 5 cells. Experimental (solid lines) vs numerical (dotted lines) temperature rise (right).

6 Summary

The goal of this work is to simulate the whole chain of cell thermal runaway events triggered by mechanical or thermal abuse from a single cell to a multi-cell configuration within LS-DYNA.

In order to do so we performed experiments within Ansys to show the whole process on a typical automotive-grade pouch cell. The different stages were presented with some details about the LS-DYNA setup, along with benchmarks between experiment and simulations.

Such a workflow could be repeated on other cell models for other EV's or hybrid vehicles.

7 Literature

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