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Finite element analysis of a lithium-ion battery cell under abuse conditions †

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Abstract: Lithium-ion battery cells are the fundamental components of all Energy Storage Systems (ESS) used in electric vehicles (EVs). Increasing concerns about safety issues, particularly the response of battery cells to mechanical crushes that can lead to internal short circuits (ISC) and potential thermal runaway (TR), necessitate detailed investigation. To evaluate the response of the battery under abuse conditions, a homogeneous finite element model (FEM) of the battery cell has been developed. The model employs a simplified representation of a battery cell where the internal properties are assumed to be uniform throughout the entire cell. A full factorial approach was utilized to determine the homogenized jellyroll material characteristics. A detailed FEM serves as a benchmark for validating the homogeneous battery model. While requiring less computational effort, the homogeneous model maintains sufficient accuracy, making it suitable for modelling entire battery packs, thanks to the reduced number of elements.

Keywords: Finite Element Model (FEM); Abuse test; Internal Short Circuit (ISC); Homogeneous model

1. Introduction

One of the main risks connected to the abuse condition of the electric vehicle (EV) and, therefore, of the battery pack as well, is connected to thermal runaway (TR), which causes an uncontrolled increase in the temperature, which leads to a further increase in the temperature and definitely to risk of fire. Abuse mechanisms, such as crush, can result in the failure of one of the jellyroll layers (the battery's internal structure), which leads to an Internal Short Circuit (ISC) and consequently causes an exothermic reaction, which eventually may initiate a TR in the battery [1,2]. The main objective of the simulations is to predict and mitigate the TR risk of the battery pack when undergoing crash scenarios (Figure 1). In order to do so, however, the first step is to design accurate, still computationally efficient single battery cell models. This research aims to build a proper homogeneous model of a single battery cell, which will be adopted for an entire battery pack system in future. The homogeneous model, described in Section 3.1, is validated through a benchmark, the heterogeneous model, developed in a previous work of the same authors. In section 2, the authors provide an overview of mechanical testing procedures per international and European standards. The results of the simulations are provided in section 4, in which the results of the proposed models are compared, and a best-fit material characteristic is proposed.

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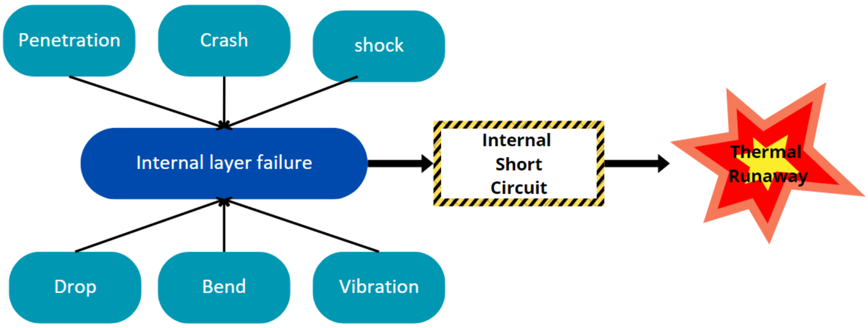


Figure 1. Schematic view of abuse events that might cause thermal runaway.

2. Overview on international standards for abuse conditions

International standards regarding abuse testing on lithium-ion battery cells are continuously evolving. These tests simulate conditions a battery might encounter during real-world use, mishandling, or accidents [3]. The main goal is to ensure that lithium-ion cells do not fail in ways that could lead to fire, explosion, or other hazardous outcomes under mechanical abuse, ensuring both safety and reliability. Table 1 provides an overview on international standards on mechanical testing, some of the most common include:

- **Impact Testing:** Simulates a heavy object falling on the battery.
- **Crush Testing:** Applies force to compress the battery, simulating situations where a battery might be crushed.
- **Penetration Testing:** A nail or other sharp object penetrates the battery, mimicking damage from punctures.
- **Vibration Testing:** Tests how batteries respond to sustained vibration, replicating conditions in vehicles or machinery.
- **Shock Testing:** Exposes batteries to sudden acceleration or deceleration, like what might happen in a crash.

Table 1. International standards overview on mechanical testing.

	International						**EU**	**USA**			**China**
Test	**SAE J2464 (2021)**	**SAE J2929 (2022)**	**IEC 62660-3 (2022)**	**ISO 12405-4 (2018)**	**ISO 6469-1 (2022)**	**UN 38.3 (2023)**	**UN/ECE R100.2 (2022)**	**UL 2580 (2022)**	**US-ABC (2022)**	**Freedom-CAR (2020)**	**GB 38031 (2020)**
Mechanical shock	C M P	C M P	C	P	C M P	C	C M P	C M P	M P	M P	
Drop	P	P			C M P	C		C P	P	P	C
Penetration	C M P				P	C			C M P	C M P	C P
Immersion	M P	P			P			M P	M P	M P	
Crush/Crash	C M P	P	C		V	C	C M P	C M P	C M P	C M P	C P
Rollover	M P	P						P	M P	M P	
Vibration		C M P	C	P	C M P	C	C M P	C M P	C M P	C M P	P

The main tests considered and replicated in simulations in this work are the impact and indentation tests. The first one consists of a cylindrical indenter posed on an orthogonal position to the battery under test (BUT) and then is impacted by a drop weight that strikes the indenter and, therefore, crushes the BUT [4]. The letter test (one of the most common in literature [5–8]) consists of an indenter that hits the cell with a certain velocity. These tests have been simulated and replicated in the heterogeneous and homogeneous models to compare the results.

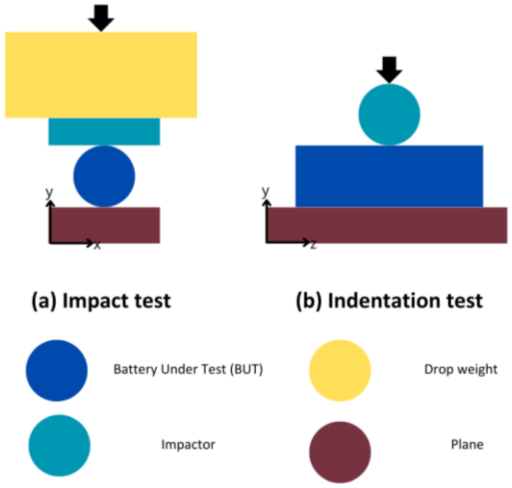


Figure 2. Schematization of an impact and indentation test.

3. Battery cell finite element models

Several numerical models have been proposed in the literature to simulate battery cell behaviour under abuse conditions [9–11]. Homogeneous and heterogeneous models are the two main categories. The multilayer jellyroll structure is reduced to a continuous, uniform material with averaged attributes in the homogeneous models [9]. On the other hand, by precisely modeling every layer inside the jellyroll structure, heterogeneous models offer a more accurate description [10]. By capturing the mechanical interactions between the layers, these intricate models hope to provide insights that more closely resemble behavior seen in the actual battery. Their primary benefit is their great accuracy, especially when it comes to locating short circuits and recognizing localized problems like mechanical failure in particular layers [11]. Furthermore, these models are more accurate in forecasting how safe battery cells will be under different abusive scenarios. When compared to homogeneous models, their main disadvantage is the increased computational expense and implementation complexity.

Nevertheless, the authors develop a homogeneous model in this work, using a detailed heterogeneous model as a benchmark case study. The heterogeneous model has been developed in a previous work [12], which is in the publication phase, and will support the homogenization process by working as a benchmark case study since an experimental test campaign cannot be performed due to safety-related concerns. The simplified model will be calibrated using the detailed model results, and the jellyroll's material characteristics will be studied to fit the heterogeneous model results best. Both battery cell models have been developed within the explicit dynamic solver Ls-Dyna V971 R10.1.

3.1. Development of a homogeneous battery cell model

The internal structure of a li-ion battery cell comprises a layer of anode and cathode compound (both made of a metallic current collector coated on both sides with active material) separated with a permeable membrane referred to as separator. This entire stack is then tightly rolled and this is why it is also referred to as "jellyroll" [13]. The thickness of each layer of separator is in the order of ~µm, whereas the electrodes compound (anode and cathode) thicknesses are in the order of ~10^2 µm. The material usually adopted are depicted in Table 2 below. In this case a commercial 18650 NMC battery cell was replicated.

Table 2. materials of the layers.

Layer	**Material**
Cathode electrode compound	
Current collector	Aluminium
Active material	NMC/NCA/LFP/LTO
Anode electrode compound	
Current collector	Copper
Active material	Graphite
Separator	PP/PE
Case	Stainless steel

Nevertheless, the internal layered structure of the jellyroll implies some difficulties. First of all, the small thickness of the elements, associated with a radial evolution of the jellyroll, means that the mesh elements adopted have big aspect ratios and critical time steps. Moreover, the number of nodes in the model are extremely high, in the order of $\sim 10^6$ which results in single simulation requiring more than 20 hours to be computed. Considering all this, it is clear that a detailed heterogeneous model cannot be adopted in a full battery pack crush simulation to represent single battery cells. If we consider a Tesla Model S battery pack, for example, it utilizes a total of 7104 cylindrical 18650 battery cells [14]. This would rise the number of nodes to more than 10^9 just for the cells, not considering all the envelops. This is why detailed heterogeneous model cannot be used in large scale simulations.

In order to model a full battery pack the first step is the homogenization of the jellyroll with a consequent reduction of the number of nodes. A homogeneous jellyroll model assumes uniform material properties and a single, consistent material representation [10], as it can be seen in Figure 3. This kind of simplification drastically reduces the calculation time needed for the simulation but also the modelling effort and is suitable for large-scale simulations. On the other hand, it lacks in terms of accuracy and has a limited insight of the internal localized phenomena undergoing inside the battery cell.

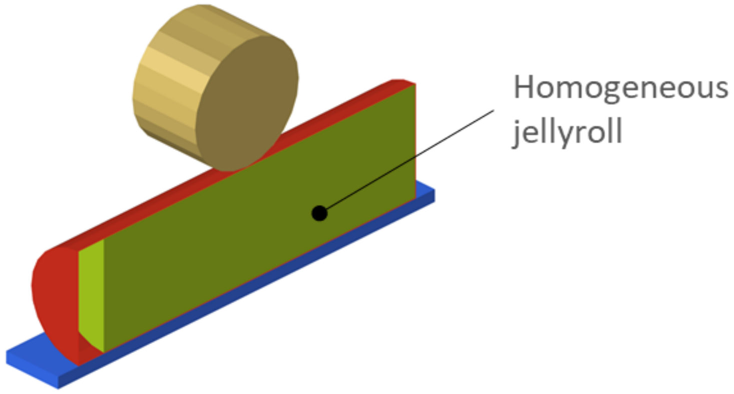


Figure 3. Schematization of the homogeneous jellyroll model.

This work aims to build accurate yet simplified homogeneous jellyroll material characteristics that can replicate the results of the detailed model within an acceptable accuracy range, based on the root mean square error (RMSE).

3.1. Homogeneous material model

The material model utilized by the authors is largely adopted in literature and is derived from [10]:

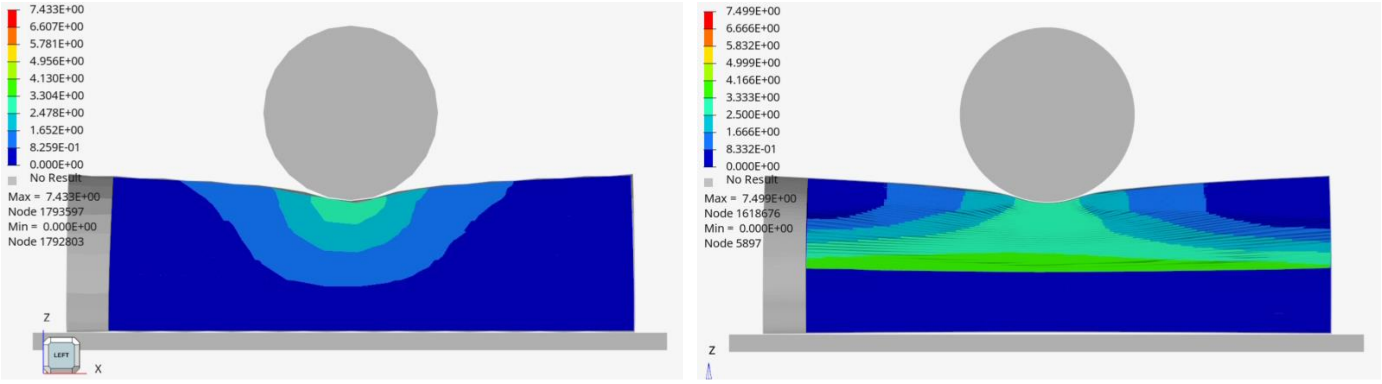
$$\sigma = A\varepsilon^{B} \tag{1}$$

In this equation, A and B represent two parameters which would need to be calibrated through the experimental campaign on a stack of jellyroll material. In this work, authors calibrated the parameters adopting a full factorial approach, simulating all the possible combinations of A and B within a predefined range:

- A = [1000:1000:10000]
- B = [1:1:5]

The simulation was automatically run using a script that generated all the key-files needed for the LS-Dyna environment.

The simulations were run for the indentation and the impact test, considering the same range, for 50 simulations each. The time required for a single simulation is less than 1 minute, drastically reduced compared to the 20 hours of the heterogeneous model. The number of elements of the homogeneous model is reduced to ~10^3, which means we obtained a 3-order reduction. Figure 4 shows a comparison between the simulation results of the homogeneous model (left), and the heterogeneous model (right).



(**a**) (**b**)

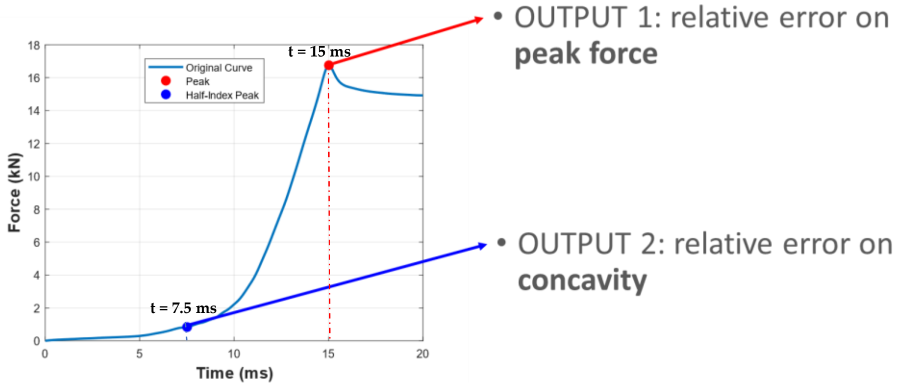
Figure 4. Comparison of the two proposed model: (**a**) Homogeneous model; (**b**) Heterogeneous model.

4 Simulation results

In order to evaluate the simulation results, two output parameters were defined:

1. Peak force: relative error on the peak vertical force.
2. Concavity: relative error on the vertical force considering a point halfway to the peak force. This parameter was conventionally called concavity by the authors, even if it is not a proper concavity but it works as an indicator for the lower part of the curve, characterized by lower forces and displacements.

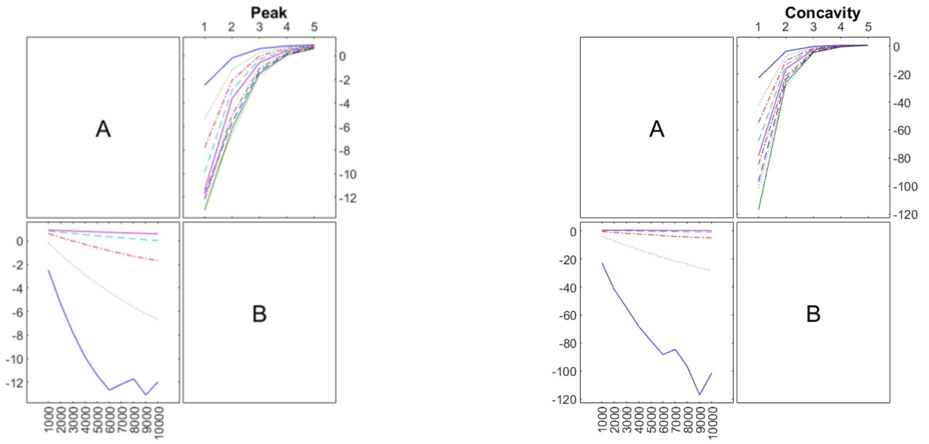
For each simulation, A and B's influence and interaction with the results were evaluated to understand the best range of A and B so that a more refined study can investigate the value of best fit with an even greater degree of accuracy.



- OUTPUT 1: relative error on **peak force**
- OUTPUT 2: relative error on **concavity**

Figure 5. Simulation output.

The results are shown in Figure 6 and Figure 7. For both indentation (Figure 6) and impact (Figure 7) tests, the first outcome is that B has great relevance on the relative error for both peak force and concavity: the value of B should be in the upper limit of the range (B = 4 or 5) to reduce the relative error. Independent of the A value, B should significantly reduce the error if a higher value is taken into consideration. Let us consider the influence of the A parameter. It is evident that the influence of A is less evident when the B value is higher: if we observe the fourth quadrant, the blue curve refers to B=1 and the pink line to B=5; we can assume that higher the B value, lower the influence of A. Nevertheless, lower values of A are to be considered if B is lower.



(**a**) (**b**)

Figure 6. Comparison of the two output parameters in the indentation test: (**a**) peak force; (**b**) concavity.

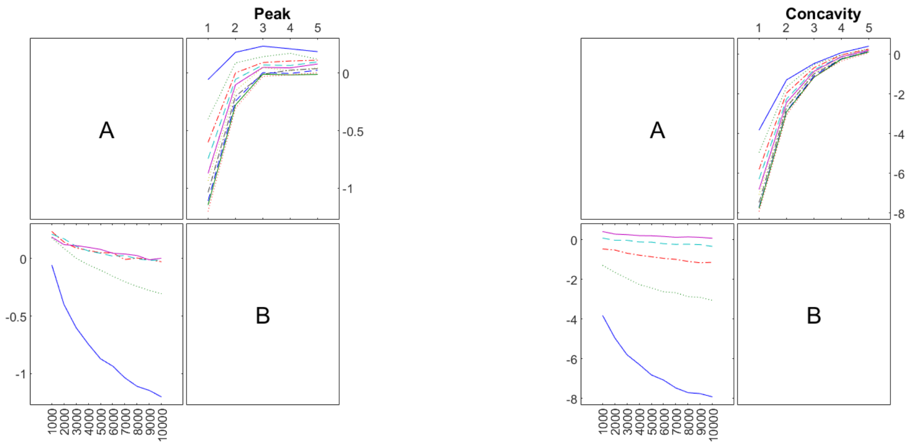
4.1. Best fit for jellyroll material: a single model

The main output of this research work is developing a material model that can be used in a finite element model of a battery pack. Once the influence of the two parameters is understood, the best fit for each test case was analyzed based on the RMSE evaluation. In Table 3, some of the RMSE values of the simulations are shown. The best RMSE values obtained were in simulation R039 and R049 for impact and indentation, respectively. The response in terms of vertical displacement for the impact test is visible in Figure 8, where the benchmark curve (in orange) is plotted.

Moreover, if we sum the RMSE for the two simulations, the minimum RMSE sum is on R039, which is the best fit for the indentation test and works well for the impact test (yellow curve). Material characteristics in terms of A and B parameters can be used to simulate both indentation and impact.

Table 3. Some of the RMSE values of the simulations in both test cases. The red ones are the best fits in terms of RMSE for each test.

Version	RMSE_Impact	RMSE_Indentation	Sum
R001	5.3	29.5	34.8
R006	7.3	60.3	67.6
R011	7.9	86.3	94.2
R017	4.8	30.7	35.5
R023	1.8	6.4	8.2
R028	2.2	9.1	11.3
R034	0.8	2.4	3.2
R039	0.5	1.3	1.8
R042	6.3	64.3	70.6
R048	3.4	17.3	20.7
R049	0.6	0.7	**1.3**



(**a**) (**b**)

Figure 7. Comparison of the two output parameters in the impact test: (**a**) peak force; (**b**) concavity.

In conclusion, considering the results obtained, the authors decided to employ the features of R049 in homogeneous models. In addition, the results highlighted that homogeneous models are potentially a solution that can effectively replace the use of detailed models.

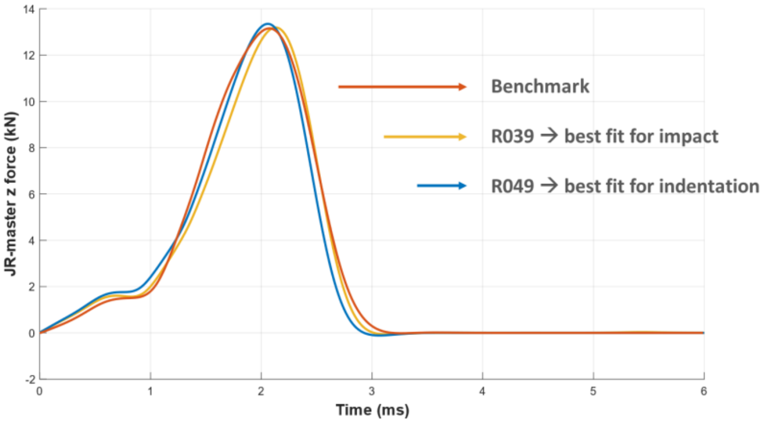


Figure 8. Best fit curves for the two tests, applied to the impact test simulation.

5. Conclusions

Simulations play a crucial role in predicting and reducing the risk of thermal runaway during crush testing. An accurate yet simplified model of the battery cell, known as the homogeneous model, is needed to simulate an entire battery pack effectively.

The authors introduced a homogenization process using a full factorial approach to simulation, which generated a best-fit curve for the battery's response. For validation, they compared the simplified homogeneous model to a detailed heterogeneous model they had previously developed. It was found that a single material model can be used in both test scenarios (indentation and impact).

Therefore, in this paper, a unified material characteristic was proposed. It can be applied across multiple test cases, eliminating the need for a specific material for each test.

This model represents a significant step toward future advancements in battery pack modelling.

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