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Failure Prediction of Railway Battery Cells Under Large Deformations

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Abstract

Batteries are a key component for developing innovative battery and hybrid multimodal trains that are currently candidates to substitute Diesel Powered Rolling Stock on non-electrified or partially electrified lines. Also, on conventional rolling stock, innovative high-performance batteries can contribute to weight lightening or ensure a higher and more reliable backup power for auxiliaries. Due to their extremely high energy content, innovative lithium batteries also introduce a potential risk of fire in case of thermal runaway or in case of crash-induced deformations able to cause internal short circuits. Failure phenomena associated with internal breakdown and short circuits involve modelling very small-scale phenomena associated with the non-linear strain of deformation of the internal thin layers of cells. In this work, authors focus their attention on finite element modelling techniques that should help to properly simulate and predict the strain-induced cells of batteries and how these results can be exploited appropriately to produce simplified or surrogate large-scale models that can be very useful to extend the study to large scale battery packs.

Keywords: lithium battery, large deformation, structural failure, finite element, thermal runaway, battery-operated trains.

1 Introduction

Hybrid, battery-operated, or fuel cell-propelled rolling stock represents a feasible alternative to diesel-powered rolling stock on non-electrified or partially electrified lines. All these different kinds of multimodal propulsion systems can be treated as suggested by regulation in force [1] as particular subcases of a more general architecture of hybrid series system described in Figure 1: all the subsystems that compose the propulsion layout are treated as primary power sources, storage systems and loads converging to a common power node. This system's conceptual design corresponds to an equivalent implementation in which this power-sharing node is physically represented by a constant voltage DC bus, which is connected to over-cited loads, sources, and storage. Often, connected subsystems cannot share directly with the DC bus since associated internal voltages are different, so intermediate static converters are introduced to manage both reversible and irreversible power flows. In terms of equivalent bond graph modelling [2,3], the system is composed of sources (the primary power sources) connected to capacitive (batteries and or capacitors) and resistive (substantially all the loads) elements connected to a common junction through transformers (as an example, static converters) and gyrators.

Batteries are a key component of this different propulsion configuration, serving alternatively as main power storage (as an example in battery-operated trains) or as power buffers (as an example in hybrid systems). In both cases, the size of installed batteries in terms of equivalent nominal power and energy are relevant (from several hundreds of kWh to several MWh). Also, in conventional rolling stock, considering a mean consumption of auxiliaries from 25 to 35 kW for each coach, the size of installed backup batteries should be quantified in at least 10-30kWh/coach, so also, in this case, the total installed capacity on a medium composition of 8-10 coaches can be in the order of hundreds of kWh. The energy density of conventional lead-acid batteries installed on coaches is about 40Wh/kg, so the evolution to lithium batteries with higher energy density levels (from 100 to 300 Wh/kg) can contribute to reducing the weight of installed batteries of hundreds of kilograms or even tons according to the investigated train compositions.

Despite the development of more stable and reliable cell chemistries such as LiPO4 or LTO, there is a potential fire risk associated with large deformations that should occur on cells and batteries in case of accidents. Regulation in force also for the railway sector [4,5] describes tests including shock prescriptions for different storage systems. However current technology development

The authors focus on finite element modelling techniques to accurately simulate and predict the deformations induced in battery cells. In particular, the complex mechanical behaviour of battery components and how these modelling approaches can effectively capture it is studied. By evaluating the accuracy of strain prediction within cells, researchers can gain valuable insights into the structural integrity and performance of battery systems.

In addition, the authors explore how these simulation results can be exploited to develop simplified models suitable for analysing large-scale battery packs. These simplified models retain the essential features of detailed models while reducing computational complexity, enabling efficient analysis of larger battery systems. By extrapolating knowledge from cell-level detailed model simulations, researchers can improve understanding of behaviour and build increasingly faithful equivalent models. Overall, this approach facilitates a more comprehensive assessment of battery pack performance and safety, enabling engineers and researchers to optimise design parameters and operational strategies to improve reliability and efficiency in various applications.

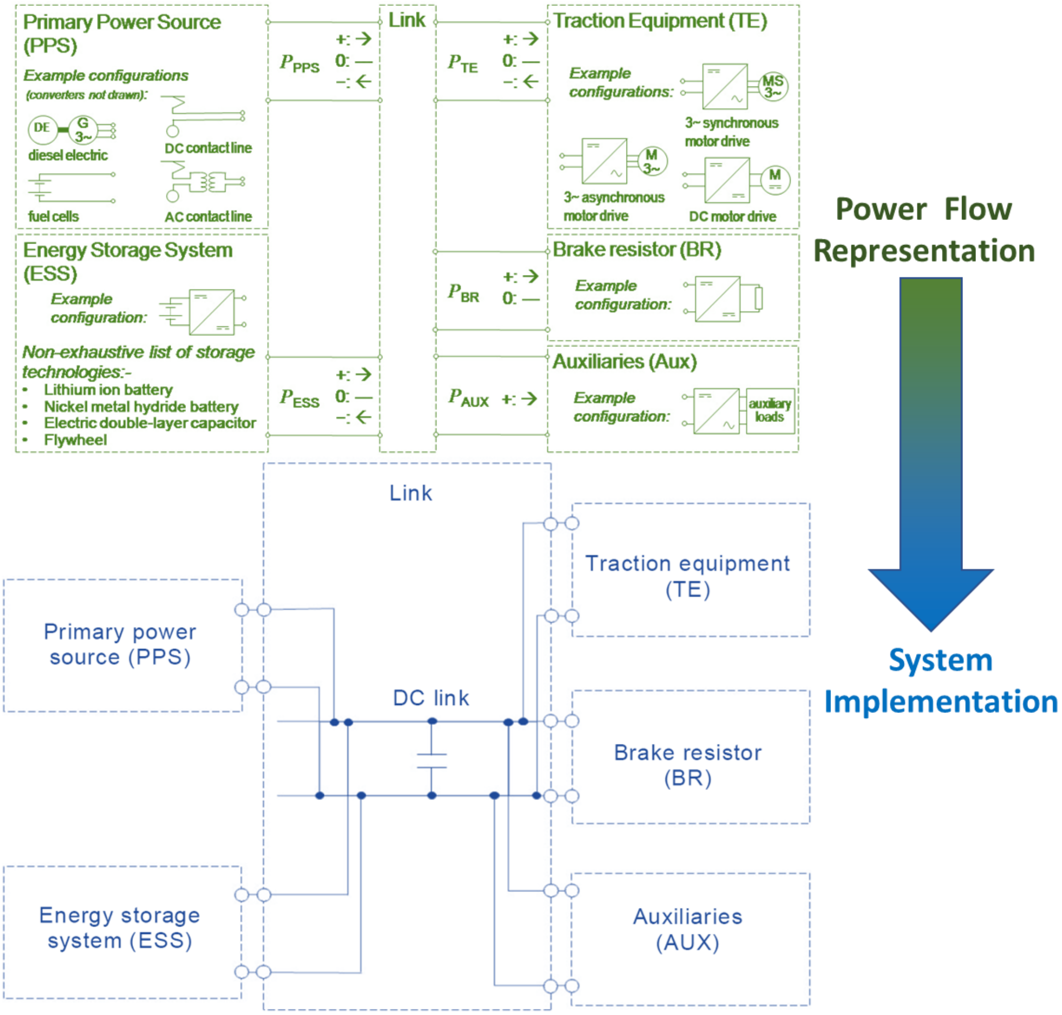


Figure 1: Multimodal hybrid series trains from power flow representation to corresponding system implementation [1].

2 Methods

This section describes the approach used in the different stages of the activities. In section 2.1, the state of the art regarding the internal layout and structural behaviour of battery cells, mainly focusing on the role of the separator between the anode and cathode in the occurrence of internal short circuits, is examined and discussed. Moreover, a brief investigation of the FE models for lithium-ion battery cells proposed in the literature is presented. Finally, section 2.2 introduces a finite element model of the battery cell, explaining the modelling and materials approach used and a qualitative validation of the results compared with those found in literature.

2.1 State of the art

The battery cell jellyroll consists of layers of a positive electrode (cathode), a separator, and a negative electrode (anode). At a more granular level, each electrode includes a metallic current collector coated with the active material on both sides. The specific materials and chemistries used for the various layers are detailed in the Table 1. In section 2.2 the model developed considers the whole electrode compound, so the jellyroll consists of a repetition of the anode-separator-cathode unit stack.

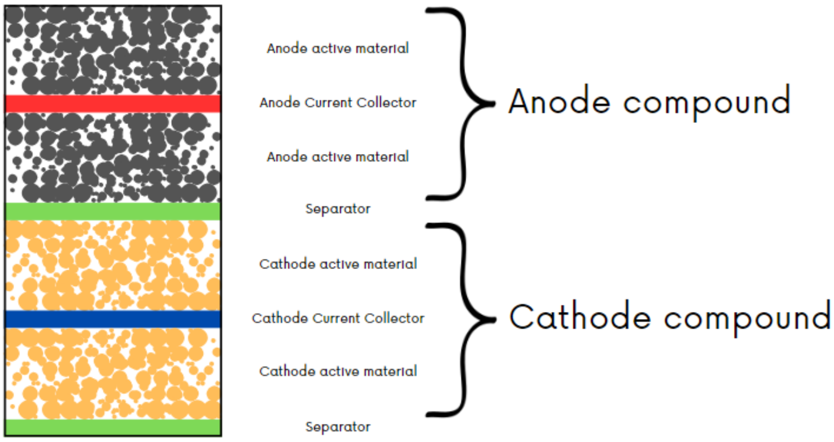


Figure 2: Elementary layered structure of a lithium-ion battery cell.

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

Table 1: Materials usually found for the jellyroll layers.

The separator layer, composed of a porous polymer, isolates the positive and negative electrode compounds while facilitating Li-ions transport through its porous structure [6-7]. This layer plays a critical safety role within the jellyroll configuration, as any failure of the separator and subsequent contact between the electrodes can initiate an internal short circuit (ISC), potentially leading to catastrophic events such as thermal runaway [8]. Therefore, the separator must endure significant deformations without failing. Studies have demonstrated that during abuse testing, the active material of the electrodes is the first to crack, whereas the separator exhibits substantial resistance to deformation before eventually fracturing [9].

Abuse testing of a battery cell involves subjecting it to extreme conditions to evaluate its safety, performance, and reliability. These tests, for example, include bending [10], penetration [11], and indentation [12] of the battery cell (see Figure 3). They are performed to evaluate the battery behaviour in crash scenarios and are representative of such events [13].

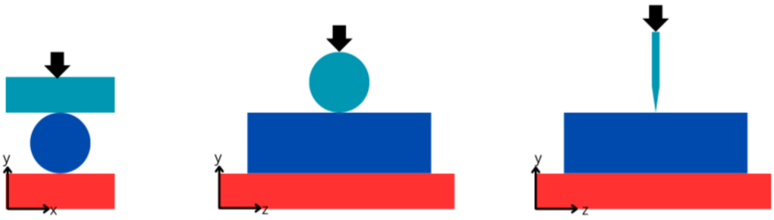


Figure 3: Abuse testing scenarios: (a) compression, (b) indentation, (c) nail penetration.

Among those, the indentation test is one of the most commonly performed in literature [14, 12, 15] and is suitable for representing side impact scenarios of an EV. At the cell level, tests are usually performed using a cylindrical impactor, whose diameter is comparable to that of the battery under test (BUT). The force-displacement response of the BUT is captured and is then used to evaluate the onset of ISC and validate the numerical model.

In order to replicate the battery cell behaviour under abuse conditions, few numerical models have been proposed in the literature [14, 12, 9]. The main models are the homogeneous and the heterogeneous models. The layered jellyroll structure is approximated in the homogeneous models as a continuous, homogeneous material with averaged properties [14]. On the other hand, heterogeneous models provide a more accurate representation by explicitly modelling each layer within the jellyroll structure [12]. The detailed models aim to capture the mechanical interactions between different layers, providing insights closer to real-world behaviour. The advantages of the detailed model are mainly related to their high accuracy in providing detailed insights into localised phenomena, such as mechanical failure at specific layers and, therefore, the short circuit location [9]. Moreover, these models are more accurate in predicting the safety performance of the battery cell under different abuse conditions. The main drawback lies in their high computational cost and implementation complexity compared to the homogeneous models.

Nevertheless, the authors develop a detailed model in this work not only to have a better insight into the battery cell failure mechanisms but also to serve as a benchmark for the future development of homogeneous simplified models.

2.1 FE model description

The authors developed a finite element (FE) model according to [12] within the explicit dynamic solver LS-DYNA V971 R10.1. The cell was discretized into four key components: casing, separators, and homogenised cathodes and anodes. Other cell components were neglected due to their minimal influence on structural response.

The casing utilises shell elements with an elastoplastic (piecewise isotropic) material law. Solid hexahedral elements with a crushable foam material law model the separators, anodes, and cathodes (refer to Figure 4 for the normalised compression-tension behaviour versus volumetric strain). Both anodes and cathodes were homogenised, treating the active material and current collector as a single entity.

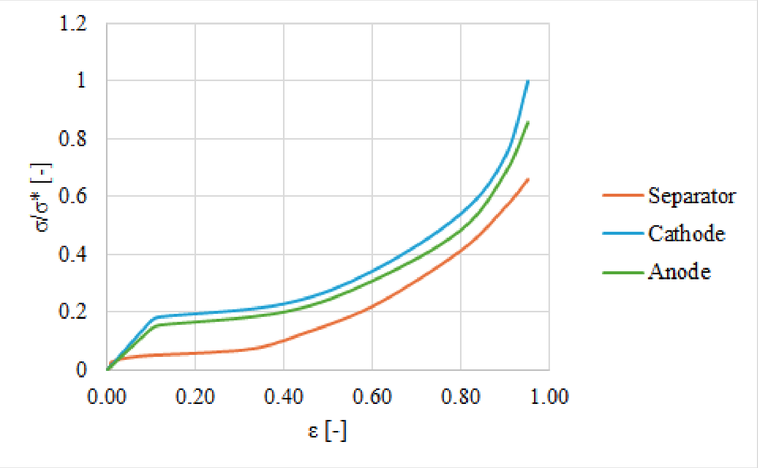
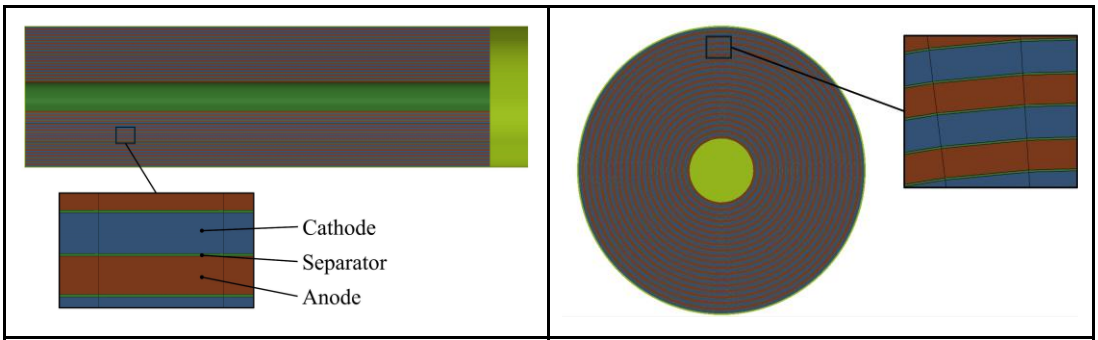


Figure 4: Normalised compression stress vs volumetric strain for anode, cathode and separator.

From a geometric perspective, the cell represents an 18650 battery layout, with the internal helical layering simplified to axial symmetry (Figure 2 (a)). Additionally, the meshes of the separators, anodes, and cathodes are constructed to facilitate contact in a curved geometry (Figure 2 (b)). The boundary and coincident nodes between layers are not merged to allow for delamination. An internal segment-based contact (automatic single surface) with static and dynamic coefficients of 0.2 provides interaction between the layers. The total mesh comprises 1,500,000 nodes and 790,000 elements.



(a) Sagittal cross-section.

(b) Transversal cross-section.

Figure 5: Mesh of the battery cell.

The simulation replicates a quasi-static penetration test: the cell is placed on a support plate and crushed with a cylindrical impactor until reaching a penetration depth of 7.5mm. Due to limited computational resources, the model does not include strain rate effects, so we apply time scaling to the impactor velocity. A velocity of 0.5m/s is chosen to neglect inertia effects [12]. Both the plate and the impactor are modelled as rigid materials. The whole model (Figure 6) consists of 1,690,000 nodes and 890,000 elements.

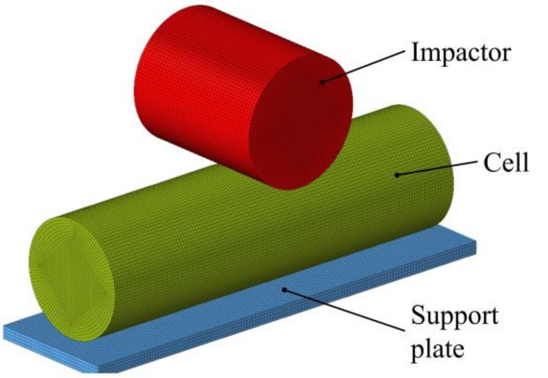


Figure 6: Model of quasi-static penetration test.

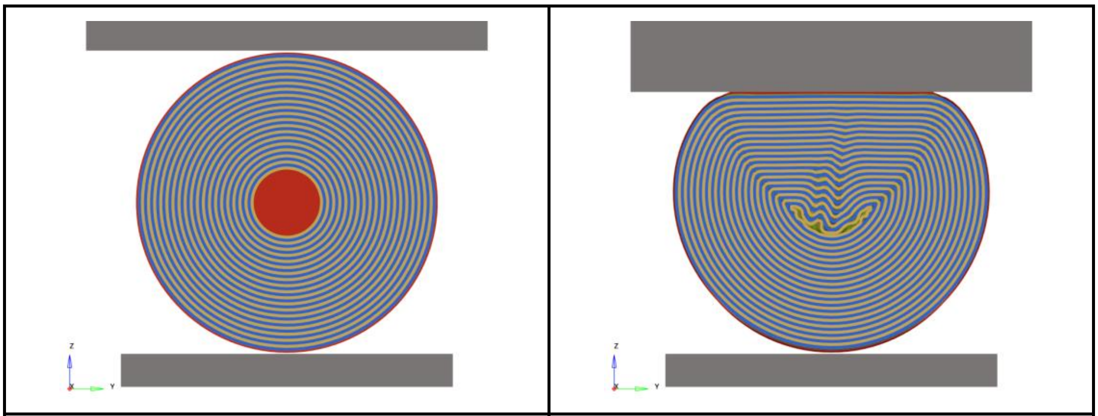
Since no specific experimental data is available, the authors used the results from the literature as a broad benchmark to evaluate the model's predictive capability. Therefore, the validation process relies more on a qualitative approach than a quantitative one, assessing whether the model can reproduce the mechanical response and identify points of most significant stress, such as those that could lead to separator failure, at similar locations.

3 Results

In the following section, the results of the indentation test simulation are reported and analysed. The time needed to solve the model using LS-DYNA mpp971 single precision is approximately 20h computed on a server with 72CPUs.

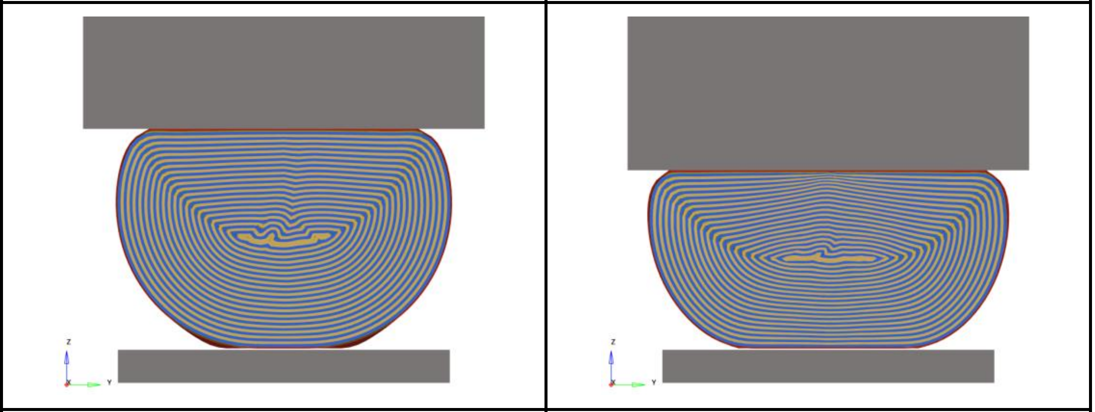
As mentioned in the previous section, the FE model is created with the guidelines and characteristics identified in [12]. Therefore, the validation mainly follows a qualitative and only marginally quantitative approach.

Figure 7 reports the animation frames in the transversal section at four equidistant impactor displacement *d* values. At 2.5 and 5.0mm impactor displacements, a deformation of the inner layers comparable with literature can be observed [12]; the upper zone (impactor side) of these layers collapses downward, resulting in a self-contact with the lower part.



(a) d=0.0mm

(b) d=2.5mm



(c) d=5.0mm

(d) d=7.5mm

Figure 7: Animation frames in transversal section cut.

Even the sagittal section at the ultimate impactor displacement (Figure 8) shows delamination of the inner layers comparable with the deformations found in literature [9, 11, 12].

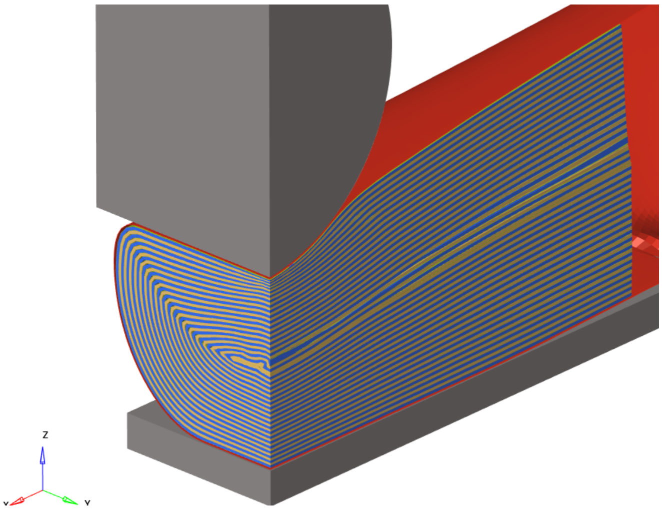


Figure 8: Sagittal section cut.

The analysis is focused on the separator, considering its role in internal short circuits; the von Mises stresses and equivalent plastic strains of the separator are illustrated in Figures 3.2 and 3.3, respectively. In most cases, failures of the separator are the primary causes of internal short circuits, making these metrics critical for understanding its structural integrity and durability.

Figure 9 (a) shows the distribution of von Mises stresses across the separator, highlighting regions where the stress is concentrated. Higher von Mises stress areas are more susceptible to failure, potentially leading to an internal short circuit.

Figure 10 (b) presents the equivalent plastic strains within the separator. These strains indicate permanent deformations when the material is under stress beyond its elastic limit. Regions with high equivalent plastic strains indicate areas where the separator has undergone significant deformation, increasing the likelihood of failure.

By examining these figures, we can identify the stress concentrations and deformation patterns points (A) and (B) that may compromise the separator's effectiveness, ultimately leading to internal short circuits as described in the literature [9].

The last validation phase involved (Figure 10) a comparison of the output force-displacement of the impactor with corridors elaborated from data reported in [12]; in particular, *Spielbauer Corridor* approximately represents the area between numerical and experimental data of specific cells. In contrast, *a Generic Corridor* approximately represents the area across different cell types. The force-displacement resulting curve (red) does not precisely match the corridor, but the overall behaviour and ultimate force are comparable.

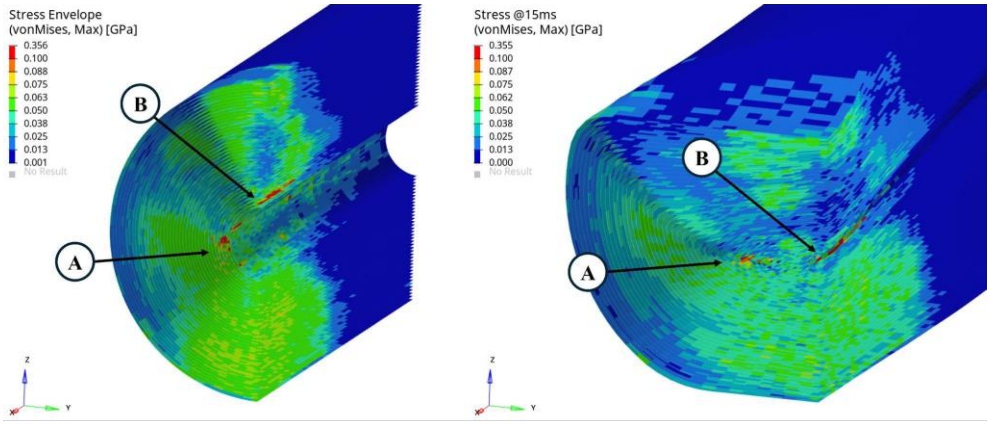


Figure 9: Von Mises Stress (Envelope and last time of simulations).

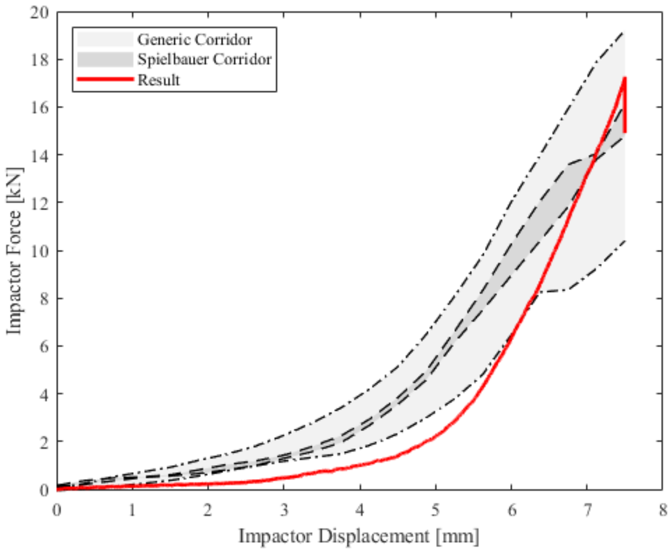


Figure 10: Force [kN] versus Displacements [mm] of impactor.

4 Conclusions and Contributions

This study presents a detailed finite element (FE) model to simulate the mechanical behaviour of a cylindrical 18650 battery cell under quasi-static loading, focusing on the separator's role in internal short circuits. By replicating the jellyroll structure and implementing comprehensive material properties and contact interactions, the model captures mechanical responses and failure mechanisms observed experimentally in literature.

The FE model enhances our understanding of battery cell failure mechanisms and serves as a benchmark for developing simplified homogeneous models. It highlights stress concentrations and deformation patterns that can lead to separator failure and internal short circuits, crucial for improving battery safety and reliability in railway applications.

Despite its high computational cost and complexity, the model's accuracy in predicting localized phenomena and safety performance under abuse conditions makes it vital for lithium-ion battery research. Future work will optimize the model's efficiency, expand its application to various battery designs and loading scenarios, develop methods to predict internal short circuits and validate the model with experimental data.

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