Abuse Characterization and Simulation of Battery Cells Using Layered Approach

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1 Introduction

The adoption of electric vehicles (EVs) has brought renewed attention to battery safety, particularly in scenarios where batteries are subjected to mechanical abuse, such as car crashes. The potential for battery cells to catch fire or exhibit thermal runaway under such conditions necessitates a comprehensive understanding of the underlying physics. The complex interplay of structural, thermal, electrical, and electrochemical phenomena presents a formidable challenge for accurate simulation and prediction of battery behavior. In this context, the integration of multiphysics coupling within Ansys LS-DYNA® has emerged as a crucial tool for studying battery abuse and enhancing safety measures.

Two distinct approaches can be used when modeling battery cells using Ansys LS-DYNA®. The first is a homogenized approach, known as the BATMAC model, which uses an equivalent circuit representation of the cell. This model is favored for its computational efficiency, enabling swift simulations. This is particularly relevant for crashworthiness assessments, where swift analyses are paramount. However, its use of homogenized material representations for the cathode, anode, and separator may limit its ability to capture nuanced localized phenomena. On the other hand, the layered model adopts a more detailed approach. Each layer of the cell – cathode, anode, and separator – is meticulously separated, allowing for the examination of local cell failure.

This paper will present the workflow of a refined battery layered model representing each layer of the cell used during experimental tests performed by Ansys. Such a detailed model regarding the experimental results will be crucial in our understanding of the different local phenomena that cannot be captured by BATMAC and will help improving the workflow that Ansys LS-DYNA® offers for the battery simulations in full vehicle crashes.

2 Materials and Methods

2.1 Battery cell abuse tests

The battery abuse test conducted by Ansys involved a commercially available NMC/Graphite Lithium-ion pouch cell [1,2]. The cell dimensions were 200mm x 150mm x 7.38mm, composed of 25 unit stacks, resulting in a total thickness of 7.38mm. Each unit stack's specific composition was determined through the analysis of computed tomography (CT) data (Table 1).

Component	Material	Thickness
Positive Current Collector	Aluminum	0.016 mm
Negative Current Collector	Copper	0.010 mm
Positive Electrode	NMC	0.067mm
Negative Electrode	Graphite	0.045 mm
Separator	Triroll (PP/PE/PP)	0.025 mm

Table 1: Battery unit stack structure.

The battery cells were subjected to various loading cases to validate and calibrate its mechanical properties. Battery cells were fully discharged before performing the mechanical abuse experiments to prevent batteries from going under thermal runaway scenarios. The battery cells were subject to four different test cases: flat punch compression, medium hemisphere indentation, rod indentation, and small hemisphere indentation (Table 2).

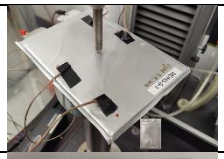
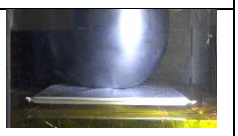
Flat Punch Compression	Medium hemispherical indentation	Rod indentation	Small hemispherical indentation	Large hemispherical indentation
Ø: 40 mm	Ø: 25.4 mm	Ø: 15.6 mm	Ø: 12.7 mm	Ø: 150 mm
Battery discharged	Battery discharged	Battery discharged	Battery discharged	Battery fully charged
				
				

Table 2: Experimental setup [1,2].

An additional test was carried out on a battery at 100% state of charge (SOC), utilizing a 150-mm hemispherical indenter in order to record both the electrical and thermal reactions of the battery cells (Table 2). The results revealed that, shortly after the hemisphere indentation, the battery cell entered a state of thermal runaway.

2.2 Battery cell model

The computational mesh of the cell was generated using the Battery Packaging option within Ansys LS-Prepost (Fig. 1). The cell's multilayer mesh, consisting of 400000 solid elements, was created due to restriction from the Multiphysics solver with fully integrated elements. An 8-point hexahedron intended for elements with poor aspect ratios (**ELFORM -2**) was chosen as it provided an accurate representation of the cell's complex geometry without an excessive computational cost.

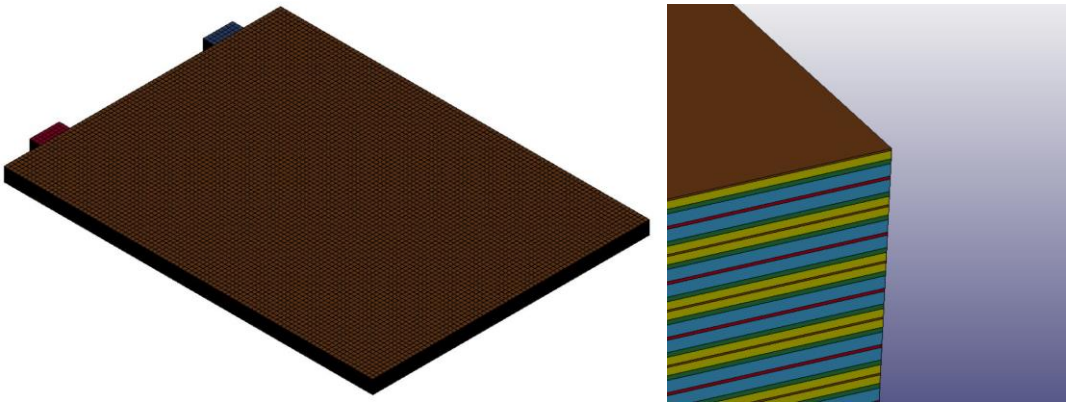


Fig.1: Battery cell model

Initially, the simulation encountered a negative volume error, a common issue when using finite element methods to model highly deforming structures. To mitigate this challenge, the battery mesh was adapted to closely match the shape of the indenter. Additionally, the utilization of eroding single surface contact played a crucial role in updating contact interactions during deformation, further enhancing the reliability of the simulation results.

Material properties were assigned to various battery components. Aluminium and Copper properties were defined as ***MAT_PIECEWISE_LINEAR_PLASTICITY** and **MAT_ADD_EROSION** using Ansys Granta Selector®. NMC, Graphite, and Separator properties were defined as ***MAT_CRUSHABLE_FOAM** and **MAT_ADD_EROSION** using pertinent literature [3] except for the separator's properties determined through an optimization process on the flat punch test due to the difficulty to obtain compressive material properties.

The indenter used for each simulation was considered rigid, with a prescribed displacement applied until battery failure (usually observed at 50% of compression).

2.3 Multiphysics

Cell electrical properties represented by Randles Circuit parameters were generated from the Hybrid Pulse Power Characterization (HPPC) test conducted by Ansys [1]. Electrical conductivity and thermal properties for all battery components were incorporated based on data from Ansys Granta Selector® and relevant literature [4].

Randles Circuit model mimics the electrothermal response that happens within the cell [5]. In the event of the cell's internal shorts, some of the Randles circuits are replaced by a short resistance. The initiation criteria for the short circuit within the cell model are predicated on two significant factors: the mechanical failure of the separator and the melting of the separator due to temperature escalation. The mechanical failure of the separator is implemented directly through its thickness and element elimination. Concurrently, the melting of the separator is modeled by detecting if its temperature surpasses a specific threshold causing the insulation to be stripped off within the unit cell. ***EM_RANDLES_SHORT** using ***DEFINE_FUNCTION** was used to represent the separator failure and melting of the separator. Exothermal reaction models were also added using ***EM_RANDLES_EXOTHERMIC_REACTION** to simulate the rapid temperature rise during the thermal runaway event.

To manage computational expenses, the mechanical solver was frozen after reaching maximum compression and only the electromagnetic and thermal solvers were active during the internal shorts and thermal runaway events.

2.4 Solver improvement

A solver improvement allowed the initiation of a short circuit only after element deletion for a specific component (in this case, the separator), in contrast to the previous approach which allowed it for any component. This enhancement, available in version DEV-101543, offered greater simulation precision.

3 Results and Discussion

The simulations were conducted using 256 CPU cores, resulting in a runtime varying between 3.5 hours and 7 hours depending on the loading conditions.

The simulation results were validated against the force-displacement curve from the mechanical abuse tests (Fig. 2). The resulting force vs. displacement curve exhibited a good fit with experimental data, especially for the flat punch compression and the medium hemisphere indentation (Fig. 2). For the flat punch compression, this was primarily attributed to the optimization of the separator component with respect to this test. Our analysis suggests that even if optimization of the separator material properties were applied to all scenarios, a single constitutive model capable of representing all cases does not appear to exist. Introducing separator anisotropy and strain-rate dependency might be a potential avenue for future research.

The temperature, and voltage response of the battery cell model was validated against the experimental data from the large hemispheric indentor. The temperature predictions aligned well with experimental observations, accurately predicting the timing of thermal runaway events (Fig. 3). However, slight discrepancies in the slope of temperature rise were noted. This deviation could potentially be attributed to the absence of combustion modelling and certain thermal boundary conditions within the simulation setup. An exploration into cell swelling and venting processes within thermal abuse modelling could enhance our comprehension of battery responses during extreme temperature scenarios. In terms of voltage predictions, the simulation results demonstrated good agreement with experimental data up to the point of explosion (at t=5 s).

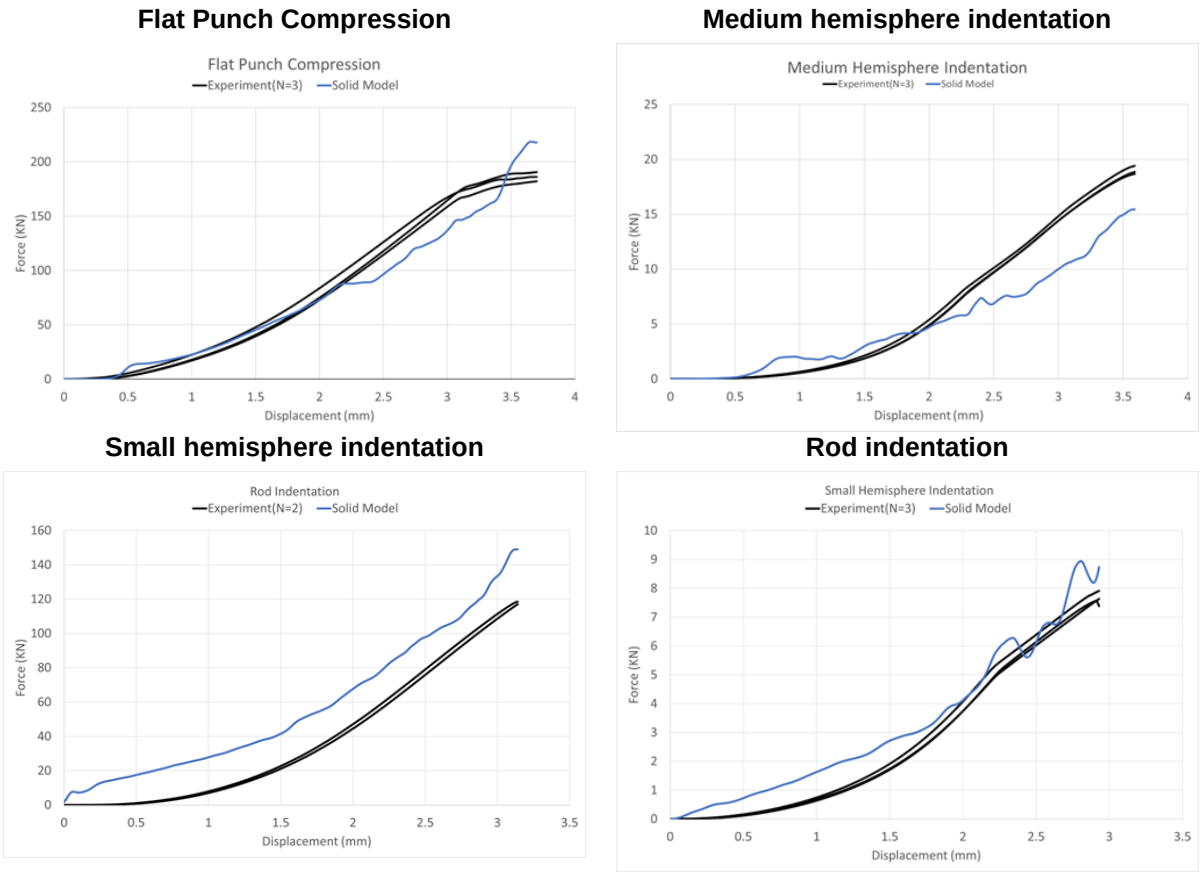


Fig.2: Mechanical abuse validation of the battery cell

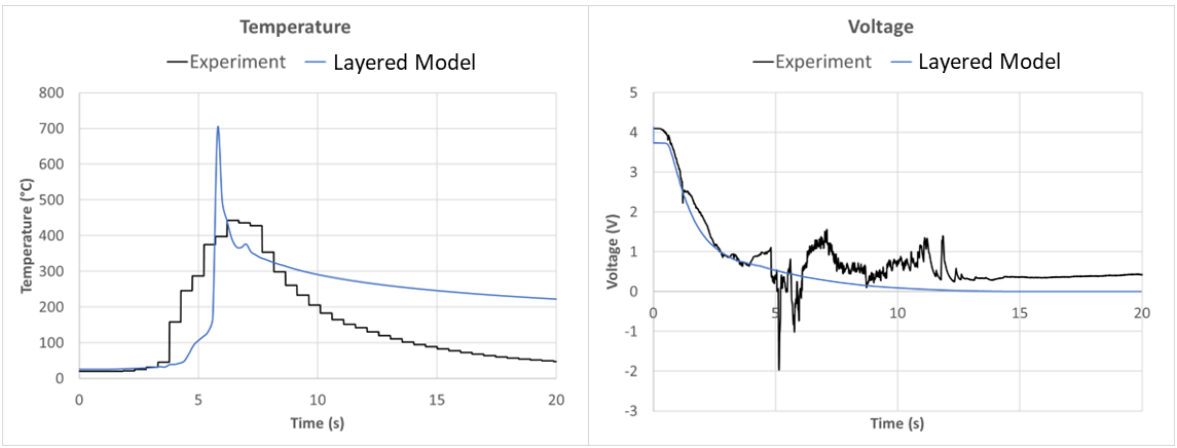


Fig.3: Voltage and temperature response during cell's internal shorts and thermal runaway in the large hemisphere indentation test

The layered model allowed to capture the progressive failure within the battery cell (Fig. 4). Consequently, a comprehensive understanding of the short progression throughout the cell's constituents was attainable (Fig. 5). Only the first eight unit stacks initiated mechanical failure in the large hemispheric indentor simulations. However, due to the battery being fully charged, this was enough to initiate the complete battery runaway as in experiments. Investigating the influence of the initial SOC on thermal runaway could yield valuable information about the interplay between SOC and thermal behavior.

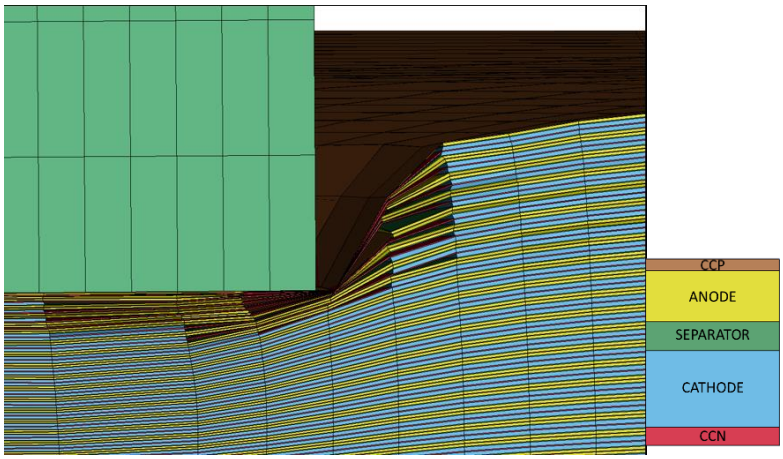


Fig.4: A cross-sectional view of the battery model with element deletion

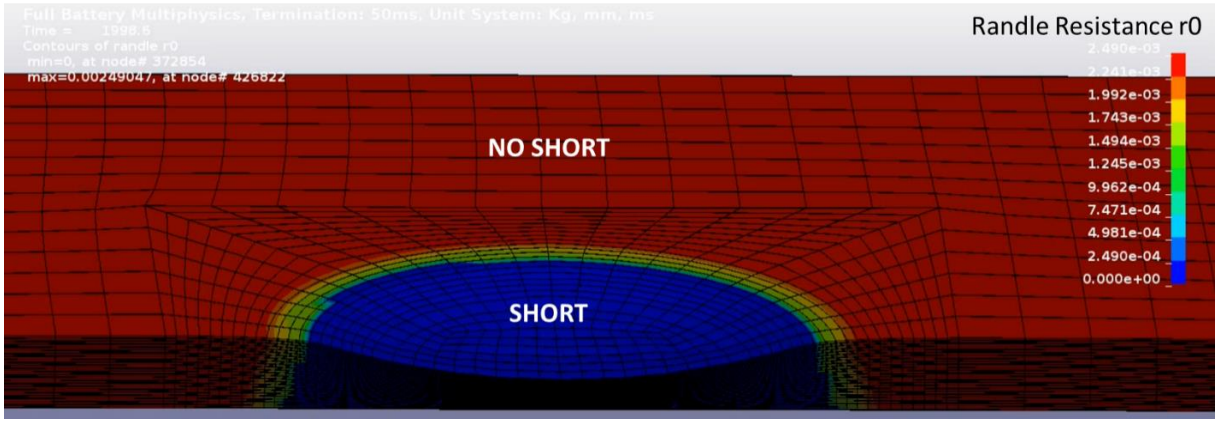


Fig.5: Randles resistance of the separator across the layered battery at t=2000 ms.

4 Summary

This paper introduces a novel method for the comprehensive modeling of battery behavior under abusive conditions, addressing complex physics couplings. The method is demonstrated through simulations of a commercially available NMC/Graphite Lithium-ion pouch cell subjected to mechanical abuse. The proposed layered model captures detailed failure responses of individual layers, overcoming limitations of existing homogenized approaches like the BATMAC model. This heightened granularity comes at the cost of computational intensity due to intricate meshing, making the layered model better suited for comprehensive cell-level analyses. Overall, this new method offers a promising advancement in battery simulation, providing insights into localized failure phenomena and enhancing the understanding of battery behavior in extreme conditions.

5 Acknowledgement

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6 Literature

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[5] P. L'Eplattenier et al., "A distributed Randle circuit model for battery abuse simulations using LS-DYNA®.", 14th International LS-DYNA® Users Conference, 2016.