Li-Ion Battery Modeling Strategies for Electric Vehicle Crash Applications

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1. Abstract

In the automotive field, car manufacturers currently face a revolution in terms of energy sources to power vehicles. The combination of electric engines and Li-Ion batteries is an efficient solution to solve environmental issues, and its usage is expected to grow in the future.

Nevertheless, this technology may present some serious hazards which origins are different than the thermal engines ones. The Li-Ion batteries are generally located all along the floor chassis and the car center of gravity is then lowered compared to other vehicles. Consequently, the safety concerns to investigate are different than usual. The short-circuit represents the greatest risk among the potential dangers observed when crushing the battery. Several physical domains (mechanics, electromagnetics and thermal) are involved, resulting in a thermal runaway that might lead to an explosion.

The project deals with simulating the behavior of a Li-ion cell during a crash with mechanically-induced short-circuit using LS-DYNA[®]. The software has the technical capability to model the battery cell crash since the mechanical, electromagnetic and thermal solvers are all implemented in the code. The modelling difficulty comes from the computing resources necessary to run the calculation. Indeed, billions of elements would be necessary to model accurately the mechanics of the jelly roll assembly by separately discretizing each of its components. This work aim is to model the mechanical aspect of the problem with the best time saving optimization, which is actually the biggest challenge.

Bending and indentation studies have been done to get results and conclude investigation leads for further work. After dealing with the modelling choices, the study of the bending cell behavior is presented using periodic conditions to model an infinite plane in the third direction. The effect of the aspect ratio according to the element formulation is at the center of this study. Then a battery cell model when subjected to a 0.1 mm/min quasi-static imposed displacement indentation test with simplifying assumptions has been done in order to create an indentation model without excessive computation time.

A previous paper realized in collaboration with Ford Motor Company R&D center, LSTC and DynaS+ named "Mechanical modelling Li-Ion cell crush experiments using LS-DYNA" has been presented at the 11th European LS-DYNA Conference 2017. Since significant improvements have been done on the thick shell element formulations, the results of that paper have been updated using the latest released LS-DYNA version R10.1. These new results lead to new perspectives regarding battery behavior modelling.

2. Introduction

In the automotive field, car manufacturers currently face a revolution in terms of energy sources to power vehicles. The combination of electric engines and Li-Ion batteries is an efficient solution to solve environmental issues, and its usage is expected to grow in the future. Nevertheless, this technology may present some serious hazards which origins are different than the thermal engines ones. The Li-Ion batteries are generally located all along the floor chassis and the car center of gravity is then lowered compared to other vehicles. Consequently, the safety concerns to investigate are different than usual. The short-circuit represents the greatest risk among the potential dangers observed when crushing the battery. Several physical domains (mechanics, electromagnetics and thermal) are involved, resulting in a thermal runaway that might lead to an explosion.

The pouch cell internal structure is made from repeated layered structures of positive electrodes (cathodes), separators and negative electrodes (anodes) that can be folded or coiled in different patterns. Electrodes consist of a layer of metal (Al, Cu) foil (current collector) usually covered on both sides with active material. The active material is very porous and saturated by electrolyte. The layers are planar sheets with length and width of up to tens of centimeters and thicknesses of the order of micrometers.

The Ford – LSTC collaboration has developed a specific 3D electromagnetic (EM) battery model. This model has been coupled with simplified mechanical-thermal model to validate the multiphysical behavior. Then, once a realistic mechanical model is developed, it will be coupled to both thermal and EM solvers in order to simulate battery cells in normal use as well as during abusive scenarios when the structure of the battery is damaged [1]. Since the cell mechanical behavior is the main modelling difficulty of the project and necessary for the calibration of the electromagnetic model, the focus of this paper is on the mechanical part.

The mechanical response of the battery cell internal structure (called jelly roll) is still not well understood. The project requires to model crush experiments using explicit solver, in particular model the mechanics of the jelly roll assembly by separately discretizing each of its components which imply significantly high computing capabilities for all but very simple problems.

Taking into account the layers thicknesses, a cell model with 3 elements in the thickness of each layer and with a ratio aspect equal to 1, would require 228 billion elements. Moreover, the size of the elements in this model must be of the order of several micrometers which would greatly diminish the time step. In addition, during the indentation test the elements are compressed and their thicknesses are then reduced. As a result, the time step decreases over time.

The combination of all these features shows that obviously, it is not feasible using an approximative 15 x 20 cm cell when complete vehicles are constituted of only several million elements of the order of a few millimeters. Thereby it is fundamental to make appropriate and smart modelling choices and use available options in LS-DYNA enabling to reduce the total computational time while ensuring a correct cell mechanical behavior.

The mechanical study and modelling of the cell subject to crush experiments can be separated into two parts. The first concerns the behavior of the battery away from impact where the only relevant mechanical stress is the bending one. This deals with the use of the best element formulation according to the aspect ratio variation on 3 points bending simulations. The aim of this approach is to find the best time saving while ensuring a correct cell mechanical behavior.

The second step of the approach is the behavior of the battery at the precise location where the cell will be impacted where the relevant mechanical stresses are mostly compression and shear stress. There is some interesting work with representative sandwich (RS) models [2, 3, 4] which validate that using a single RS can simulate reasonably well the mechanical response of a full pouch cell during indentation tests. In addition, some interesting work using thick shell element and composite formulation might permit to integrate a battery cell model into a full car crash one without greatly modifying the computational time of the assembled model.

3. Bending behaviour study

The first step of the project is to determine which element class is the best to simulate our physical system i.e. regarding the final purpose which is simulating compression of stacked thin layers.

In the simulation of thin-walled structures, Belytschko-Tsay and Hughes-Liu shell elements are widely used [5]. However, in some cases thick shell elements (tshell) or solid elements are more suitable. In our case, thin shell elements cannot give satisfactory results because shell elements cannot give us relevant strain information through the thickness.

All the models in this section will be 3-points bending models. Indeed, far away the indentation punch in the cell, the only relevant mechanical stress is the bending one. Since the material choice does not influence this sensitivity study, steel and then *MAT_PIECEWISE_LINEAR_PLASTICITY has been considered. The contact friction is unknown and has been chosen equal to 0.1 (leave the default value 0 would not be realistic). Given its plan of symmetry, only half of the models are represented (see Figure 1). A vertical displacement is imposed at 1 e-4 m/s with a total displacement of 100 μ m. Although the loading speed is much higher than the one used in a typical quasi-static experiment, the simulations are still considered quasi-static since the kinetic energy represents less than 1% of the total energy [4]. To reduce the computation time in this study, a modelling technique called "false 2D" will be used which means the bending plate is modelled with only one solid or tshell element through its width, making it looks like a beam. However, two parallel symmetry planes are situated along the "beam" sides acting like two mirrors. This allows to simulate an infinite (in its width direction) bending plate instead of a bending beam.



Figure 1 Mesh of the 3-points bending simulation for the finite element formulation study (particular case with one element through the thickness). Side view on the left. On the right, the aspect ratio is highlighted with the width difference between models)

The main varying parameter in this work is the aspect ratio. Indeed, considering the significant computation time, studying the possibility of increasing the aspect ratio far away from the indentation location (and by how much) is a requirement. Besides the aspect ratio, there are three varying parameters in this study:

- The first one is the model width, depending on the wanted element aspect ratio to ensure squared elements in-plane.
- The second parameter is the number of elements through the thickness (NET). It can vary from one to three. Then the element aspect ratio also depends on the NET. For example, for the model with 5 elements along the length, if NET equals to 1, 2 or 3, the aspect ratio is 20, 40 or 60 respectively. Because modelling thin parts require the use of several elements in the plane to maintain accurate bending behavior [6], 5 elements are the minimum number along the length in this study.
- The third parameter is the element formulation. Tshell 5 and 7 were tested and solid 2, -1 and -2 were tested.

There are no experimental data for this 3-points bending study to compare our simulation results with. However, the classical beam theory gives:

$$\frac{R}{W} = 4uE\frac{T^3}{L_r^3}\tag{1}$$

where R is the resultant force, u the deflection, E the Young's Modulus, W the width, T the thickness and Lr the length between rods.

In this study, the width depends on the aspect ratio and is not the same for all models. That is the reason why we are using the nondimensional theoretical resultant force R/W (without friction) as reference value. This value is however not completely realistic as it does not take into account friction, which should not be neglected. The numerical model considers some friction and its resultant force is then expected to be higher than the beam theory value.

4. Update of the results using the R10.1 release

This part is an update of the previous paper on the same matter [7] but using R10.1 version instead of the R8.1 LS-DYNA version.



Figure 2 Element aspect ratio study on 3-points bending simulation. Resultant force comparison between element formulations using R10.1 version

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Figure 2 presents the results of the study first part. For each element formulation the curve of the evolution of the nondimensional resultant force versus the element aspect ratio has been plotted. Each point on the graph represents a simulation. There are 12 different curves coming from the five studied element formulations combined with a varying number of elements through the thickness.

An observation is that, even for a same aspect ratio, all the nondimensional resultant force are not equal. This means that some element formulations used with a certain number of elements through the thickness are not suitable to properly represent a bending behavior. To determine which formulations are accurate or not and then which one to keep or eliminate a trust interval of resultant force is defined (see Figure 2). To build the trust interval, two bounds are needed. The lower bound is determined thanks to Eqs. (1). The upper bound is chosen thanks to solid ELFORM 2 for an aspect ratio equals to 1. All element formulations outside this trust interval are eliminated.

There are then approximately six remaining element formulations. Since only one is needed to model our system, another selective very important criterion is required. This criterion is the computation time.



Figure 3 Six finalist element formulation after sorting out those which gave unsatisfying results on 3-points bending simulation. Total CPU time and resultant force over the element aspect ratio

Several observations can be made about Figure 3. First of all, in term of computation time, solid ELFORM -1 with NET=3 and tshell ELFORM 5 with NET=3 are equivalent. However, their resultant force is not the same and tshell ELFORM 5 seems to be not stiff enough compared to the solid formulation. These models were conceived with frictional contact which explains a greater resultant force than the classical beam theory prediction. Moreover, one of the best interests in using tshell elements is their theoretical capability of needing only one element through the layer thickness, so to reduce the total number of elements in the model (and increase the minimum time step). According to Figure 3 the tshell ELFORM 5 needs 3 elements through the thickness to give a rather good resultant force. As a consequence, tshell ELFORM 5 will not be preferred to model the problem.

Regarding the two remaining solid element formulations, ELFORM -1 enables more time savings than ELFORM -2 with the same resultant force and aspect ratio according to Figure 3. This is the reason why solid ELFORM -1 will be preferred as solid formulation to model the problem.

Regarding thick shell ELFORM 7 with 1, 2 or 3 elements through the thickness, the results are very promising. When the R8.1 version was released by LSTC the tshell ELFORM 7 was not available in the manual. DynaS+ tested the formulation when the previous paper [7] was written. The results were not matching the expectations at this time since the formulation was in beta-testing. Now the results of the study have been updated using the R10.1 version and the tshell ELFORM 7 seems to match the initial expectations:

- Firstly, the results in bending are now included in the trust interval for several aspect ratios with 1, 2 or 3 elements through the thickness using the R10.1 official version whereas they were not using the R8.1 beta version with 2 and 3 elements through the thickness according to Table 1.
- Secondly, indentation simulations (material characterization tests) have been performed with this formulation and were not giving results using R8.1 beta version whereas expected results using R10.1 official version.

NET	LS-DYNA MPP version	Average nondimensionnal resultant force (N/m)	Maximum acceptable aspect ratio by computatior	Maximum structural/theoritical aspect ratio
1	R8.1 beta	11.9	15	20
2	R8.1 beta	9.2		40
3	R8.1 beta	10.7	60	60
1	R10.1	11.9	15	20
2	R10.1	11.9	30	40
3	R10.1	11.9	40	60

 Table 1 Tshell ELFORM 7 results differences between the R8.1 beta and R10.1 MPP versions on the 3 points bending simulation using 1, 2 and 3 elements through the model thickness

Following this first bending study, another one had been realized, in the previous paper [7], on the complete cell using solid elements. Taking into account previous results the element formulation -1 had been used. The model was made of stacked layers. A sequence called Representative Sandwich (RS) was repeated 16 times through the thickness with an additional anode and separator at the bottom (as observed in Figure 4). Aspect ratio getting up to 600 were then tested on that cell model. Finally, good results were obtained with a maximum aspect ratio of 200, then chosen as a maximum to be used in further simulations.



Figure 4 Mesh of the 3-points bending simulation on the complete cell for the element aspect ratio with element formulation solid -1 (particular case of the ratio aspect = 20)

Regarding the results obtained with solid elements in a first hand, and with thick shell elements in the other hand, two different modelling leads are investigated. The first one is using solid elements modelling the cell by discretizing each of the components and the second one is using tshell elements. The layers of the cell would not be represented physically with some elements but within the thick shell using its integration points. The two different strategies are presented in the following.

5. First lead - Solid indentation modelling

The purpose of this section is to model the battery cell mechanical behaviour when subjected to a 0.1 mm/min quasi-static imposed displacement indentation test using solid elements. This first modelling approach had already been used and described in the previous paper [7]. Indeed, at that time, solid elements already shown good results for both bending simulation tests and material characterization tests. At that time, Ford was involved in the project and gave us some experimental tests results that we were trying to recover numerically.



Figure 5 Schematic representation and dimensions of Ford experiment indentation tests

The model presented here is the same as before but its main characteristics are reminded (for a more detailed description we advise to look at the previous article [7]).

The model composition is presented in Figure 6. It was inspired by C. Zhang's model [4] but not with the same representative sandwich sequence. C. Zhang chose a representative sandwich made of only five stacked layers whereas we preferred to consider the representative sandwich sequence previously defined as we believed it better represented the cell internal structure.



Figure 6 Three different views of the mesh used for the indentation study

Since the model has two planes of symmetry, we only considered one quarter of the (actual in-plane) domain in our finite element model (then saving computational time). The cell edges were left free and the bottom surface of the battery model was simply supported on a rigid wall. The casing was not considered in this study, since its contribution to the mechanical response or the initiation of the court-circuit can be isolated from the response of the cell components as reported by Sahraei et al. [8]. The indenter was a 3 cm diameter cylinder modelled with solid rigid elements. The indenter was moving downward in the z-direction at a constant speed of 0.4 m/s (higher velocity than during the experimental test but small enough to avoid dynamic effect and appropriate to an explicit simulation). The contact friction is unknown and had been chosen equal to 0.1 (leave the default value 0 would not be realistic). Every layers are merged between each other.

On the model edges, far away from the indenter the element aspect ratio was approximately equal to 200. There was a progressive mesh refinement towards the indenter where the aspect ratio was around 3. This allowed to reduce the total number of elements in the model down to 130,000. Also, the mesh geometry of the cell was optimized such as to fit the indenter shape. Indeed, a nodes line was created under the indenter in order to coincide with its edge. Moreover, during Ford experiments, most of the deformation and failure occurred under the indenter edges. Then two rings were created on each side of the node line with a refined mesh.

At the time of the first article [7], Ford research team had made some observations on cell deformation and failure occurring during indentation experiments. With the idea of reproducing some of these observations, a preliminary erosion criterion had been determined and used in the model. The minimum pressure at failure was chosen and set equal to the tensile stress at failure obtained for each material during their material characterization tests.

Main issues coming from this indentation modelling were caused by the contact handling. The materials used, apart from the current collectors, have low stiffnesses making them predisposed to undergo large deformations

leading to elements inversions (negative volume). Moreover, the very high levels of compression achieved in the simulation make the contact handling really difficult. Many different contact strategies (contact type, entity selection method, penalty stiffness, soft constraint option, number of cycle between bucket sorts...) were used during the first study without success.

However, MORTAR contacts were not studied in the first article [7] (not so much used for explicit analyses at that time) and have been looked at recently. First calculations show really encouraging results, unfortunately still leading to error termination, but getting to a longer simulation time with a more stable compressive behaviour.

In LS-DYNA, MORTAR contacts handle penetration in an unique way. First, they only take into account the amount of surface truly involved in the elements penetrations so to handle it. Then they consider, for each element involved in a contact penetration, the segment shape function so to calculate the nodal forces to be used for depenetration. Second, and really interesting fact in our case, the contact pressure progressively increases as a function of penetration. The more penetrated are the elements, the higher is the contact stiffness. This evolution is not linear and can be tuned after 25% of penetration using the IGAP parameter which can amplify the phenomenon. However, this contact specificity only works up to 50% of penetration.

The preliminary results using an *AUTOMATIC_SURFACE_TO_SURFACE_MORTAR contact are shown below and compared with the ones obtained in the first paper [7]. To better see the cell compressed state the indenter has been removed on some images. As observed, for a same simulation time, the MORTAR contact leads to a much more stable behaviour. Some penetrations can still be noticed on the indenter edge, really likely due to the right-angled corner hard to handle. Using the MORTAR contact, the simulation runs significantly longer before crushing. The final state where erosion has occurred is shown in the Figure 7. The Figure 8 is looking more closely at the penetration between the cell and the indenter. The penetrations get to around 50% of penetration maximum before stabilizing and staying constant (as expected for MORTAR contacts).



Figure 7 Results using an *ERODING_SINGLE_SURFACE contact (top images – previous article [7]) and using an *AUTOMATIC_SURFACE_TO_SURFACE_MORTAR contact (bottom images) at the time for which the eroding contact simulation crashes



Figure 8 Results using an *AUTOMATIC_SURFACE_TO_SURFACE_MORTAR contact at the simulation final time



Figure 9 Penetration observed between the cell top layer (colored in pink) and the indenter (in wire) when using a MORTAR contact at the simulation final time

This new contact approach study is still in progress. For now, results are encouraging and run in about 7 hours on 28 CPUs. Some additional tests will be performed on the different available MORTAR contact options. Current simulations however tend to show that using a penalty stiffness evolving with the pressure applied on the contact elements would be a good solution to this problem.

6. Second lead - thick shell indentation modelling

Despite the improvements that have been made in terms of deformation details, total computational time and contact handling, the cost of locally modelling Li-ion cell crush experiment is still too sizable to be integrated in a full car crash model. Several hours on 28 CPUs for only a 20 x 15 cm battery cell is far too much, especially knowing that a full battery pack contains hundreds of cells. In addition, the time step in the local approach model is very low compared to usual car crash models one, which would again greatly impact the complete model computation time.

Considering the updated results obtained previously in the bending study, another modelling approach using thick shell elements appears to be promising. Indeed, the thick shell element formulation 7 now gives good

results both in bending and in indentation. Moreover, it looks like it can be used with only one element through each layer thickness. These results are even more interesting that they could be used combined with the *PART_COMPOSITE_TSHELL. This keyword enables a completely new modelling method for the cell indentation. The layers of the cell would not be represented physically with some elements but within the thick shell using its integration points.

This new modelling method presents some pros and cons. Since the layers are not physically modelled, it will not be possible to visualize micro-buckling within the cell, as well as failure. However, the potential computational time savings by using this keyword might permit to integrate a battery cell model into a full car crash one without greatly modifying the computational time of the assembled model.

This keyword provides a simplified method of defining a composite material model for thick shell elements that eliminates the need for user defined integration rules and part ID's for each composite layer. When *PART_COMPOSITE is used, section definition (*SECTION_TSHELL) and integration rule definition (*INTEGRATION_SHELL) are unnecessary. The *PART_COMPOSITE_TSHELL keyword can be used only with thick shell formulations 5 (assumed strain to capture the complex Poisson's effect - reduced integration) and 7 (full integration).

For clarity concerns, Figure 10 schematically illustrates the composite modelling (on the left side) compared to the detailed modelling of all the layers present in the cell (in the middle) and the representative sandwich modelling (on the right side).



Figure 10 Sketch of the composite modelling (on the left), the local approach modelling (in the center) and the representative sandwich modelling (on the right)

This approach study is in progress and needs some important tests to be validated. Regarding the good results obtained in the previous part using the tshell ELFORM 7 with R10.1 version whatever the number of elements trough the model thickness, few different modelling strategies can be tested using the *PART_COMPOSITE_TSHELL keyword. As for now we do not know if it is sensible to represent the full cell with only one element through the cell thickness and as many integration points as layers, or if we need one thick shell per representative sandwich (or even more)? How many integration points should be used for each layer?... Analyses on these matters will be run and compared to the results obtained with the first approach cell modelling (using solids).

Below are examples of modelling strategy that are going to be tested in order to determine which one is sensible.

- to use one element through the whole cell model thickness and implement each layer by one integration point,
- to use one element for one sequence which is repeated 16 times through the whole cell model. So, 16 elements are stacked through the thickness representing each one a representative sandwich sequence and each layer is implemented by one integration point.
- to model each layer by few integration points.

- to use more than one element through the model thickness.

Later, the objective remains to introduce court-circuit modelling by adding electromagnetic and thermic to the current mechanical model.

7. Summary

The objective of this project was to focus on the mechanical modelling of a Li-ion battery cell crash in order for Ford to later create a multi-physical model with mechanical-thermal-electromagnetic coupling. Many studies have been done to either get results or conclude investigation leads for further work.

The LS-DYNA software has the technical capability to model the crash of a Li-Ion battery cell. The mechanical, electromagnetic and thermal solvers, are all implemented in the code. The modelling difficulty comes from the computing resources necessary to run the calculation. Find modelling tricks is then essential to be able to model this phenomenon without excessive computation time. Several ones have been used in this study such as to use periodic conditions to model an infinite plane in the third direction or use mass scaling to increase the model time step. Also, to approach the behaviour of the battery by modelling the sequence that is repeated through the thickness scaled at the real battery thickness or to maximize the aspect ratio of the elements so to reduce the number of elements in the model.

The work presented in this paper is an update of a previous paper [7] realized in collaboration with Ford Motor Company R&D center, LSTC and DynaS+ named "Mechanical modelling Li-Ion cell crush experiments using LS-DYNA" and presented at the 11th European LS-DYNA Conference 2017. At this time, regarding the results of the thick shell element beta formulation 7, the most suitable lead to investigate was to model the battery cell using the solid element formulation -1 because it was the most advantageous in terms of computing time. It is used outside the area under the indenter and with a large aspect ratio going up to 200 which significantly reduces the number of elements in the model.

The results were quite encouraging but penetration issues were encountered. Current simulations however tend to show that using a penalty stiffness evolving with the pressure applied on the contact elements would be a good solution to this problem.

From the time where the previous paper [7] was written, LSTC has released the R10.1 version including officially the tshell element formulation 7 and interesting results were obtained in bending. The use of this element formulation in addition of the *PART_COMPOSITE_TSHELL keyword would enable to model the entire cell with only few elements instead of modelling the cell by discretizing each of the components. The layers of the cell would not be represented physically with some elements but within the thick shell using its integration points. The potential computational time savings by using this keyword might permit to integrate a battery cell model into a full car crash one without greatly modifying the computational time of the assembled model. Work is currently on progress through an internship within DynaS+ on this subject and further encouraging work will be probably presented at the next LS-DYNA Conference on this matter.

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