

Battery abuse simulations 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. 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 multiphysics response of external or internal short circuits can lead to optimized system designs for automotive crash scenarios.

Recently, a so called "distributed randles circuit" model was introduced in LS-DYNA in order to mimic the complex electrochemistry happening in the electrodes and separator of lithium ion batteries [1][2]. This model is based on electrical circuits linking the positive and negative current collectors reproducing the voltage jump, internal resistance and dumping effects occurring in the active materials. These circuits are coupled with the Electromagnetics (EM) resistive solver to solve for the potentials and current flow in the current collectors and the rest of the conductors (connectors, busses, and so forth). The EM is coupled with the thermal solver to which the joule heating is sent as an extra heating source, and from which the EM gets back the temperature to adapt the electrical conductivity of the conductors as well as the parameters of the Randles circuits [1]. One of the advantages of the Randles circuit model is the relative easiness to introduce internal short circuits by just replacing the Randles circuits in the affected area by a short resistance [3]. The Randles circuit model also 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 [1].

Up to now, the Randles circuit model was only available on solid elements. So the user had to create a mesh with all the layers of a cell (positive current collector, positive electrode, separator, negative electrode, negative current collector, negative electrode, separator, and so forth), and define segment sets of each of the current collectors to connect them by Randle circuits in a distributive way [1]. The construction of the case was cumbersome and the mechanical solver often presented limitations on solid elements with one very small dimension compared to the other ones due to the extreme thinness of the different layers. The mechanical deformation of a succession of stiff layers (current collectors) and very soft ones (electrodes and separators) also was a challenge.

Recently, the Randles circuit model has been extended to composite Tshells [4]. These elements promise a better and faster mechanical resolution, and make the setting of the simulations much easier for the user.

Finally, a new battery packaging environment is being developed in LS-PREPOST, helping with the setup of cell or multi-cell cases.

In section 2, we will present the new battery cell model on composite Tshell and give some first example of internal short simulations, and in section 3, we will present the new battery packaging environment in LS-PREPOST.

2 The Randles circuit model on composite Tshells

2.1 EM model

When using composite Tshells, the EM solver internally rebuilds a solid mesh with all the successive layers (positive current collector, positive electrode, separator, negative electrode, negative current collector, ...). It then creates the randles circuits between the successive positive and negative current collectors. Just as with the solid elements, in the in-plane directions, there is one current collector per node in the original user's Tshell mesh [1]. The positive and negative current collectors are treated as conductors with electrical conductivities given by the user. They are automatically connected to the tabs by constraining the tabs to have the same potential as the desired current collectors (positive or negative). Section 2.4 will give more details on how to setup a case with composite Tshells.

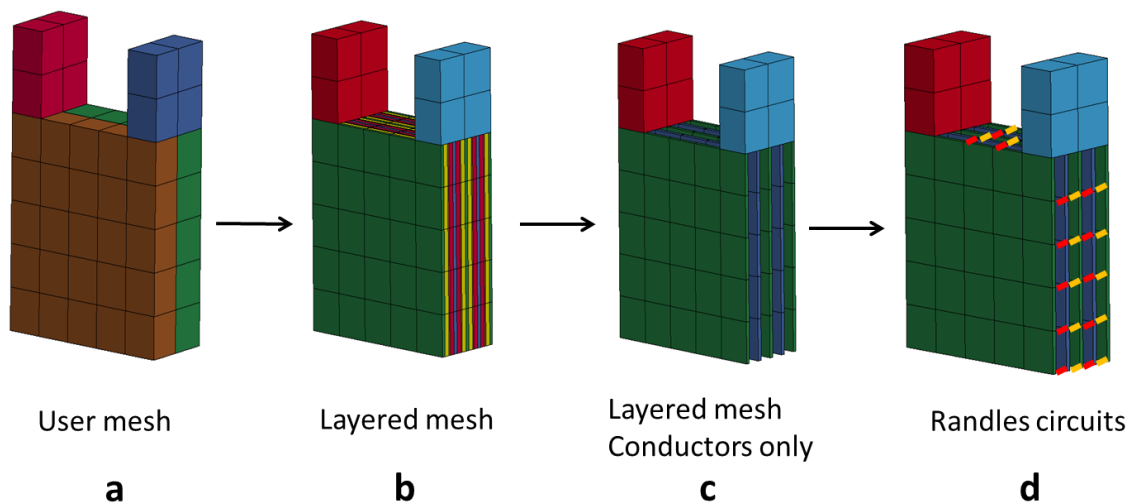


Fig.1: Illustration of the automatic building of the EM mesh from the user's mesh with thick shells (a), to the layered mesh with all the individual layers (b), to the layered mesh with only the conductors (positive and negative current collectors) (c), and building of the Randles circuit between opposite nodes on the current collectors (d).

2.2 Connection with the thermal and mechanical solvers

The local Joule heating from each Randles circuits and due to the current flow in the current collectors is sent to the thermal solver which also uses the same layered mesh as the EM solver. Equally, the temperature from the thermal solver is used by the EM solver to adjust the local electrical conductivity of the current collectors and the parameters of the Randles circuits.

The mechanical deformations of the composite Tshells induce local deformations of the layered meshes which are used to trigger internal short circuits, in the same way as presented in [1][2].

2.3 Output in LS-PREPOST

Even if the electromagnetic fields are computed on the individual unit cells on the rebuilt layered EM mesh, at this point, only through thickness averaged values are output to the d3plots. More precisely, the data represented (potential, current density, and so forth) are an average over the positive current collectors. We may extend this output to layered meshes if it proves useful.

2.4 Implementation of a case using composite Tshells

2.4.1 Creation of the mesh

We will now illustrate how to build a case on a cell that we chose to decompose as 2 composite Tshells in the thickness. Note that one can choose to decompose all the physical layers of the cell (typically around 100 for an averaged pouch cell) into 1 or as many composite Tshells as seen fit for a good resolution of the mechanical system. In all the Figures, the cell has been zoomed in the thickness direction for clarity.

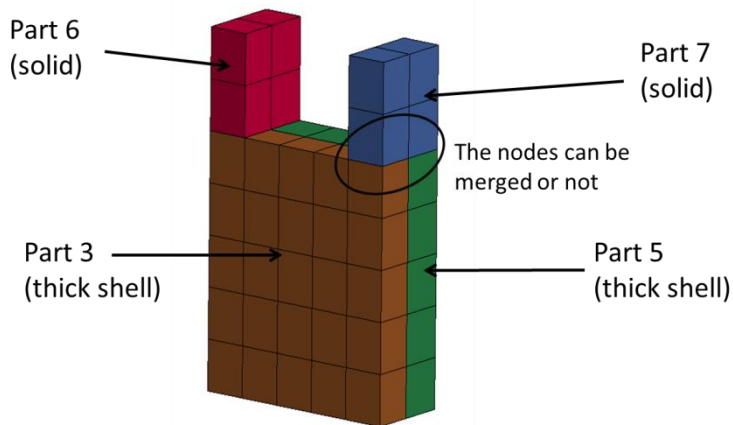


Fig.2: User's mesh for a typical pouch cell, with part 3 and part 5 as thick shells to model the cell itself and part 6 and part 7 as solid to model the tabs. The model has been zoomed in the thickness direction for clarity

2.4.2 Definition of the mechanical and thermal properties of each layer

We then define the different layers of each composite Tshell, material Id (the same material Id is used for the mechanical and the EM), thermal material Id, using the keyword ***PART_COMPOSITE_TSHELL**.

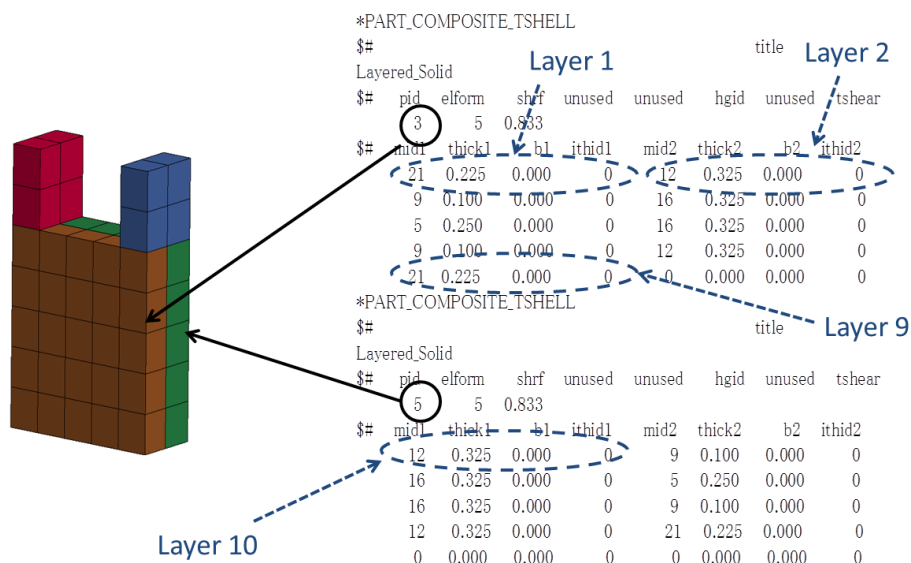


Fig.3: Definition of the different layers using ***PART_COMPOSITE_TSHELL**

2.4.3 Definition of the EM properties of each layer

One can then define the EM material type and parameters using the ***EM_MAT** cards, where an extra field "randleType" has been added to define the type of the layer. Table (1) summarizes the definitions of the randle Ids. The 2 current collectors are conductors for which the user needs to define the electrical conductivity, the electrodes and separators are insulators for the EM solver, since they are replaced by the Randles circuits. Figure (4) illustrates the setup of the ***EM_MAT** cards in connection with the ***PART_COMPOSITE_TSHELL** ones.

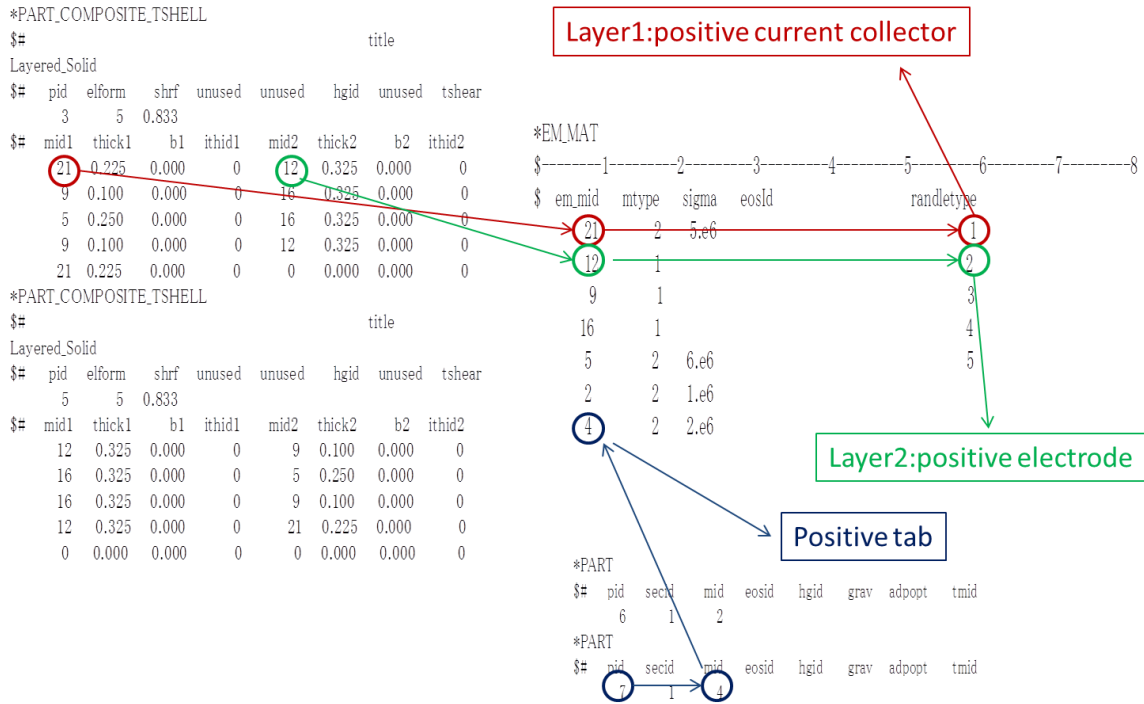


Fig.4: Definition of the EM material properties of the different layers using ***EM_MAT** cards, in connection with the mechanical and thermal definitions of the ***PART_COMPOSITE_TSHELL** cards

Layer type	randleid
Positive current collector	1
Positive electrode	2
Separator	3
Negative electrode	4
Negative current collector	5

Table 1: Randle Id associated with each layer type

2.4.4 Connections with the tabs and external circuits

In order to connect the cells with the tabs and the tabs to external circuits, the user typically needs to define the 4 node sets presented in Figure (5). Node sets 1 and 2 need to have the nodes from both the cell side and the tab side, if the mesh is not merged there.

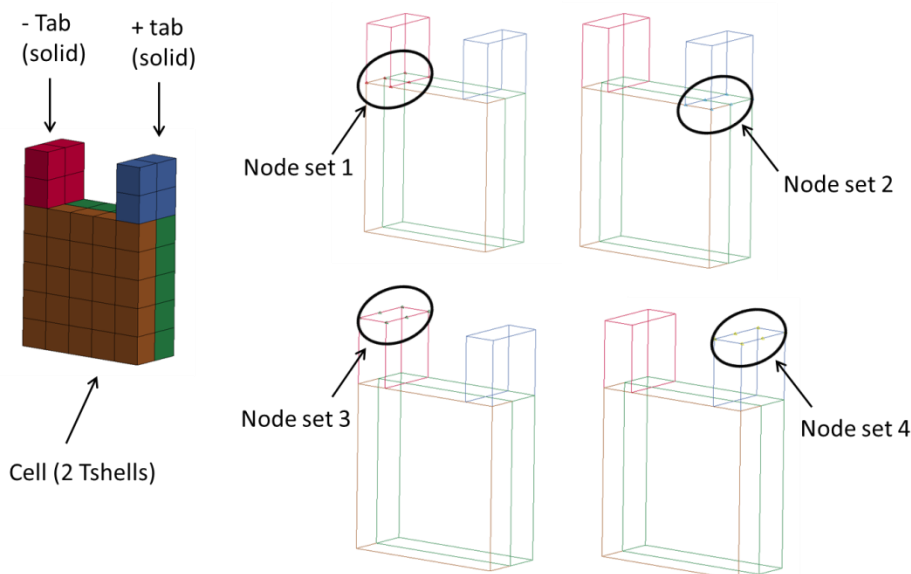


Fig.5: Node sets to be defined for the cell connection

2 isopotentials are created in order to connect the bottom of the tab with the cell. Note the new field RANDTYPE in the card, in order to specify if, on the cell side, the isopotential corresponds to the positive current collector (RANDTYPE=1) or the negative one (RANDTYPE=5) (see table (1)).

***EM_ISOPOTENTIAL**

Id	SETTYPE	SETID	RANDTYPE
1	2 (nodes)	1	5 (- curr col)

***EM_ISOPOTENTIAL**

Id	SETTYPE	SETID	RANDTYPE
2	2 (nodes)	2	1(+ curr col)

The top of the tabs can then be connected to an external circuit using the standard procedure showed in [1], using the following cards:

***EM_ISOPOTENTIAL**

Id	SETTYPE	SETID	RANDTYPE
3	2 (nodes)	3	

***EM_ISOPOTENTIAL**

Id	SETTYPE	SETID	RANDTYPE
4	2 (nodes)	4	

***EM_ISOPOTENTIAL_CONNECT**

Id	TYPE	ISOID1	ISOID2	R,V,I	LCID
1	2 (resistance)	3	4	0.01	

2.5 First examples

To illustrate the model, we now present two cases of a crash into small module. In each case, the module is composed of 10 adjacent cells mounted in parallel. Each cell, about 20 cm long, 12 cm wide and 3.5 mm thick, is composed of 22 unit cells (89 layers total, see [1] for more details on the definition of a unit cell), with 252 Randles circuits in each unit cell, hence 55,440 Randles circuit total. The user's mesh is composed of the 10 composite Tshells, each one with 228 thick shell elements. Each one of the 10 ***PART_COMPOSITE_TSHELL** thus has 89 layers. We chose very simple ***MAT** models to represent the different layers which are somehow representative of the materials but by no means optimal. Also, having only 1 thick shell for the whole 89 layers is probably not at all optimal mechanically. More research is under way to study the mechanical behavior of these complicated succession of layers with very different mechanical properties, and how to simulate them in an optimal

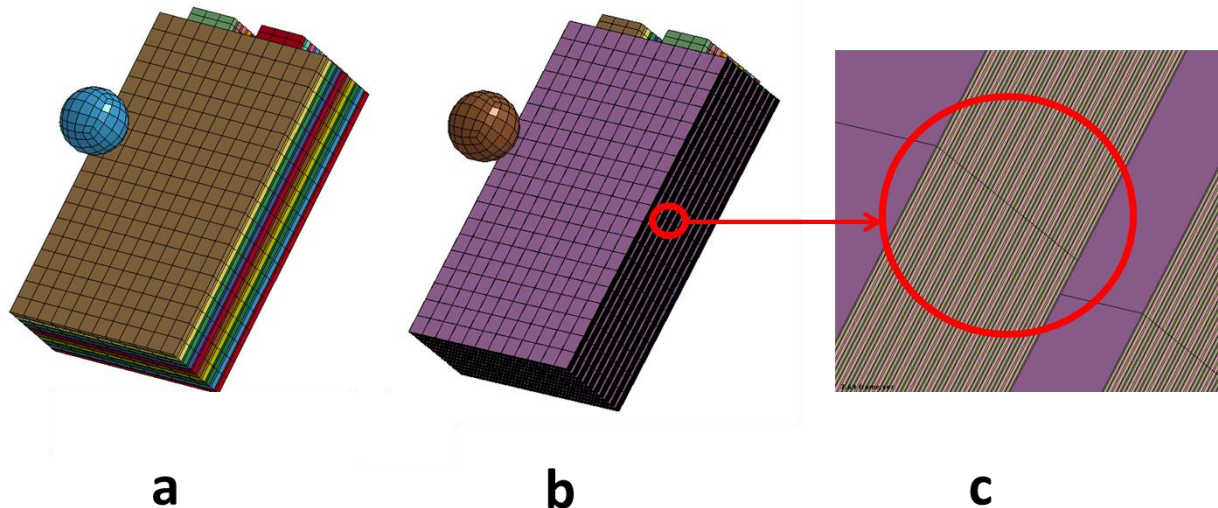


Fig.6: Sphere mesh setup. a: original user's mesh with 2925 elements, b: underlying EM mesh with 203,565 element, c: zoom on one cell of the EM mesh showing the 89 layers.

way. Here, our main goal is to show the electromagnetic capability. The underlying EM mesh for these 10 cells was composed of 202,920 elements.

In each case, the internal short circuit was triggered when the distance between the 2 current collectors defining a Randles circuit was below a certain threshold, where the Randles circuit was replaced by a pure resistance with a given value. Here also research is under way to optimize the criteria to trigger an internal short as well as the dependence of the short on some local parameters values (thickness of each electrode, separator, pressure, and so forth). The user can define the local value of the internal short resistance as a function of these local parameters by a ***DEFINE_FUNCTION**.

2.5.1 Sphere crash on a 10 cells module

In the first case, a small sphere, about 3 cm diameter, is sent against the module in a normal direction. The back and the sides of the module are constrained so that they cannot move. The sphere crashes in the middle of the module and internal shorts appear at different locations of the different cells as they get crushed enough so that the local shorts appear. Figure (7) shows the evolution of the potential and the current density as the short propagates through the thickness of the module. As explained in section 2.3, the fringe components in each thick shell is an average over all the 22 positive current collectors. This is why the potential starts with a high value (red) and decreases as the short happens, and also why the current density is not symmetric between the positive and negative tabs.

Figure (8) shows the evolution of the global State Of Charge (SOC) [1] of the module, which quickly drops from 100% to about 50% as more and more Randles circuits are shorted.

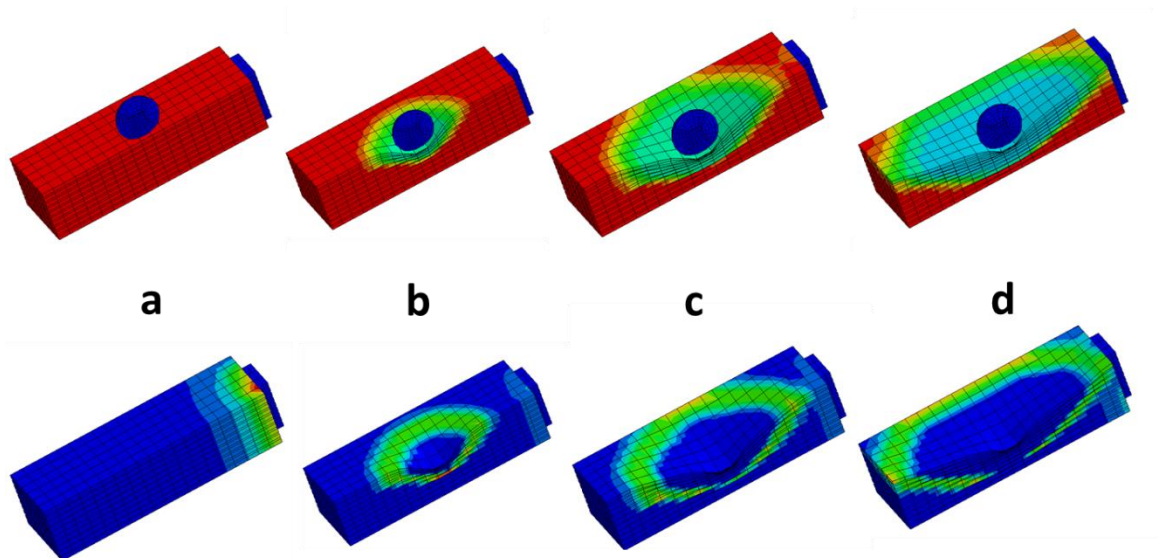


Fig.7: Impact of a sphere on a 10 cells module. Scalar potential (top) and current density (bottom) at different times of the impact: a: 5ms, b: 7ms, c: 9ms and d: 11ms. Only half of the model is represented for clarity.

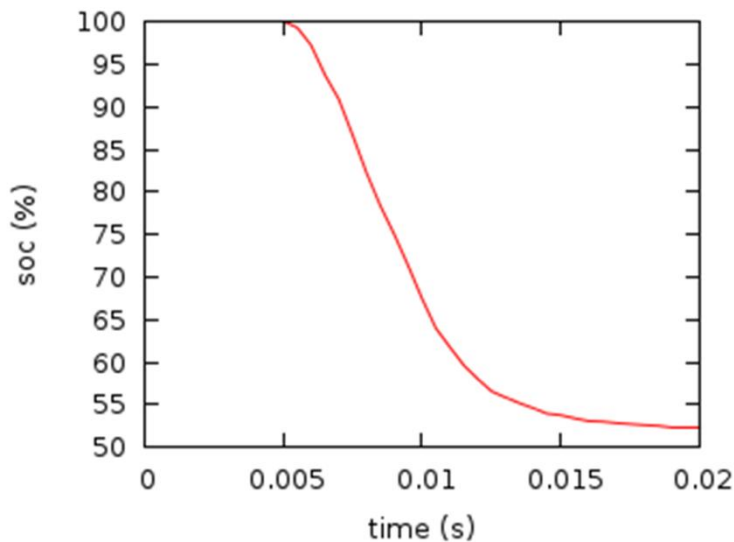


Fig.8: Evolution of the State Of Charge (SOC) of the whole module vs time during the sphere impact

2.5.2 Cylinder crash on a 10 cells module

The same numerical experiment was repeated with a 4 cm diameter cylinder oriented width-wise impacting the cell around its middle section. Figure (9) shows the user's mesh. The cells and tabs parts are the same as for the sphere case. The sphere was just changed to a cylinder.

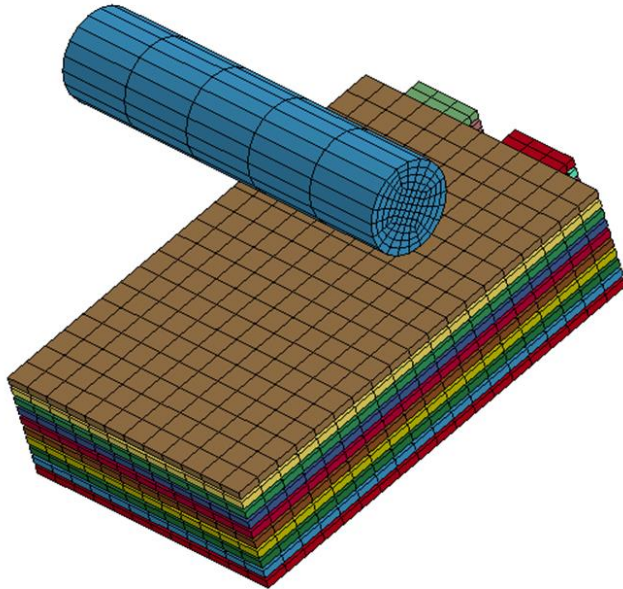


Fig.9: Cylinder crash user mesh

Figure (10) shows the potential and current density before and at different times during the impact. As can be seen, the short circuit is more severe than in the sphere case. This is because all the randle circuits which are on the other side of the cylinder compared to the tab cannot send their current to the tabs, and are thus in effect also shorted. This also can be seen in the SOC evolution plot (Figure (11)) where the SOC decreases to about 10%. This is consistent with the results presented in [3].

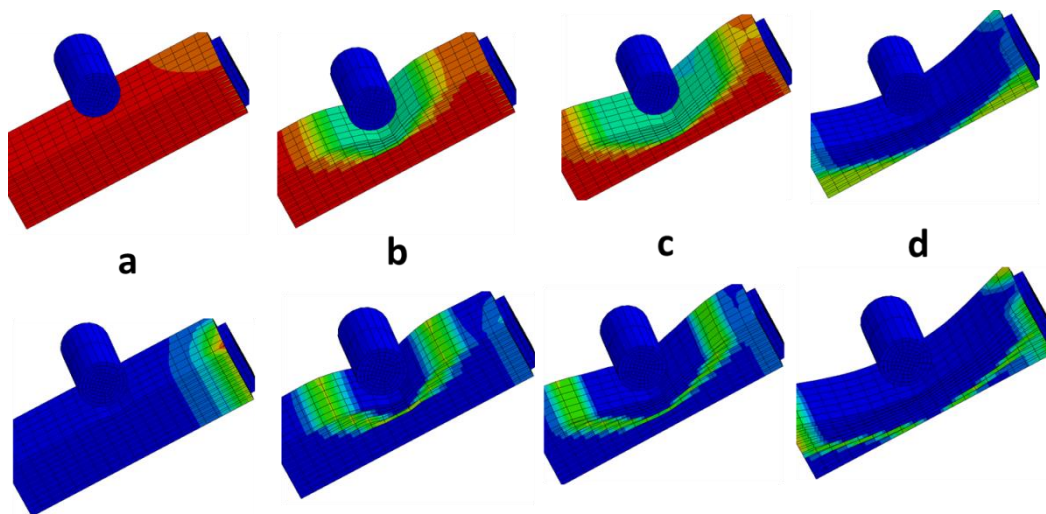


Fig.10: Impact of a cylinder on a 10 cells module: scalar potential (top) and current density (bottom) at different times: a: 10ms, b: 13ms, c: 15ms and d: 20ms

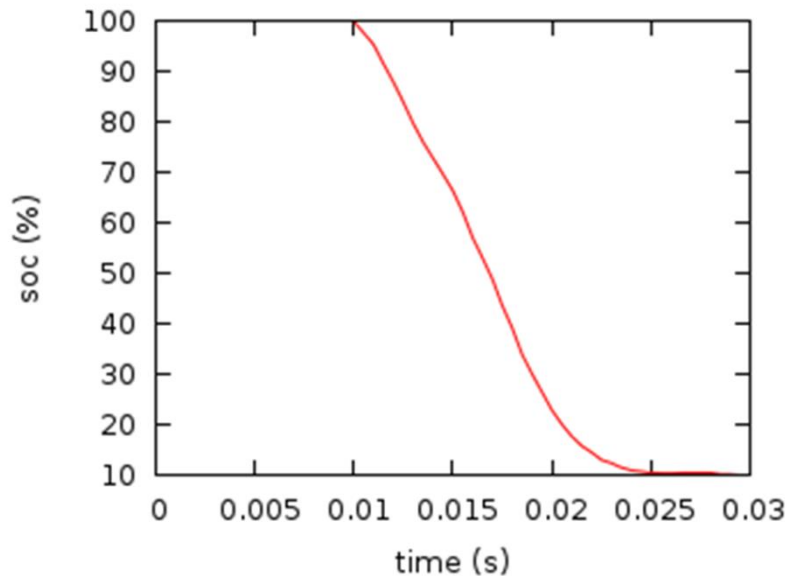


Fig.11: Evolution of the State Of Charge (SOC) of the whole module vs time during the cylinder impact

3 Battery Packaging in LSPREPOST

The latest version of LSPREPOST (LSPREPOST-4.5) includes a new interface to facilitate battery modeling development. The interface creates solid mechanical models of batteries based on pouch cells. This will soon be extended to prismatic and cylindrical cells, as well as to composite Tshells.

3.1 Overview

The new packaging can be found in Application>BatteryPackaging.

The setup of a battery model proceeds in five steps: setup of the cell, definition of the randles circuits parameters, setup of the positive and negative tabs, multiplication of the cell to create modules, and creation of the electrical connections between the cells. The definition of all the parameters are saved in the corresponding keywords. Figure (12) illustrates the setup of a battery model through the following steps:

3.1.1 Cell Setup (Figure 12-a)

The creation of the battery model naturally begins by defining the cell through its dimensions and its mesh. To define the mesh, the user just has to enter the desired number of elements in the length and in the width of the general cell. In a second step, the user defines the number of layers of the battery as well as the thicknesses and types of each layer (positive current collector (CCP), positive electrode, separator, negative electrode or negative current collector (CCN)). Finally, the user may define the material and its thermal properties of each layer.

An option allows to easily multiplying the defined layers in order to obtain a multiple layers model, such as a succession of CCP-posElec-Sep-negElec-CCN-negElec-Sep-posElec-CCP-posElec-...

Note that the packaging will group all the layers of a same type in one part. For example all the CCP layers belong to part 1.

3.1.2 Randle Circuit

The second step consists in defining the Randle circuit parameters [1], which are stored in a ***EM_BATTERY_RANDLES** card. See the manual for more details.

3.1.3 Tabs (Figure 12-b)

The third step is the setup of the positive and negative tabs. As for the cell setup, the user has to enter the desired dimensions, numbers of constitutive elements and type of material for each tab. Each tab is defined as a new part.

3.1.4 Multiple Cells (Figure 12-c)

In order to define a module or a pack, the user may, in this fourth step, multiply the cell already built along with its tabs, specifying the direction of the reproduction and the gap between 2 successive cells.

3.1.5 Connection (Figure 12-d)

Finally, the user can connect the different parts of the battery thanks to four types of connection: short, resistive, voltage or current [1]. The connections are made by defining node sets, linking them to isopotentials and using isopotential connects [1].

Figure 12-d represents the connection between the isopotential created at the top of the positive tab and the isopotential created at the top of the negative tab, allowing a defined current flow. The first two isopotentials connect the tabs to the cell.

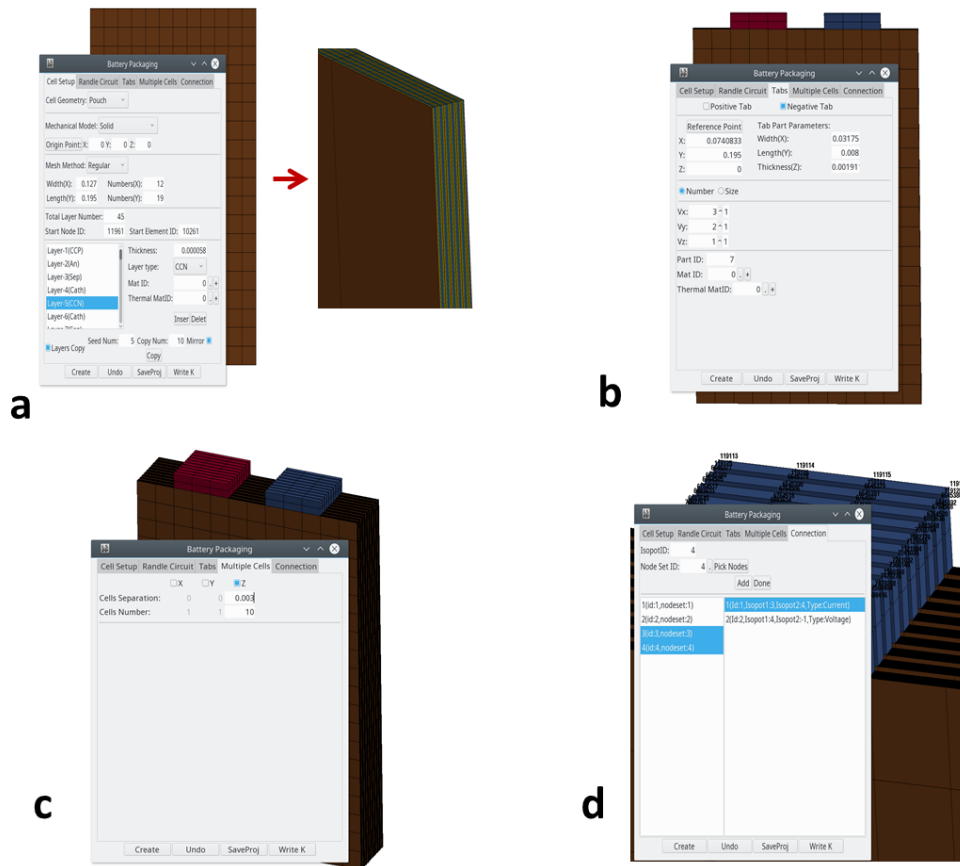


Fig.12: Different stages in the construction of a battery model using the new LS-PREPOST battery packaging module. (a): cell setup, (b): connection tabs setup, (c): going from one to multiple cells, (d): connecting the cells to the tabs and the tabs to external circuits

3.2 Model example

Through the previous steps we built easily the mesh presented on Figure (13). The insertion of the Randle circuit parameters and the creation of connection activate and manage the model, so that the model is nearly ready to run.

The next steps will be to improve the packaging by the insertion of the composite Tshells as well as other cell geometries, such as cylindrical and prismatic.

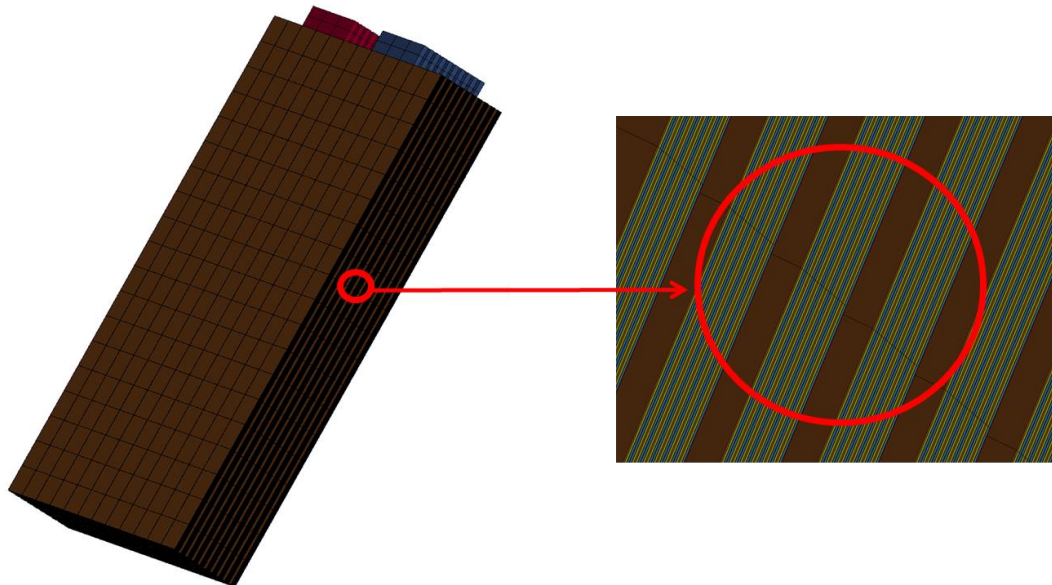


Fig.13: Mesh of a battery model – a ten cell model with 55-layers in each cell

4 Summary

The extension of the Randles circuit model to composite Tshells was presented. These new elements promise a better and faster mechanical resolution, and make the setting of the simulations much easier for the user. First internal short example using these composite Tshells were presented. Research is now underway to optimize the models in order to correctly render the mechanical deformations of these composite layers during a crash, as well as to connect them with the appearance of internal shorts and the values of the internal short resistances. The coupling with the thermal solver also is nearly completed.

Finally, a new battery packaging environment in LS-PREPOST was presented. This environment still is under development but already is available to users in LS-PREPOST-4.5 .

5 Literature

- [1] L'Eplattenier, P et al: "A distributed Randles circuit model for battery abuse simulations using LS-DYNA", 14th International LS-DYNA Users Conference, Dearborn, 2016
- [2] Marcicki, J et al: "Battery abuse case study analysis using LS-DYNA ", 14th International LS-DYNA Users Conference, Dearborn, 2016
- [3] Marcicki, J et al: "A simulation framework for battery cell impact safety modeling using LS-DYNA", Journal of the Electrochemical society, **164** (1) A6440-A6448, 2017
- [4] Chatiri, M et al: "An assessment of the new LS-DYNA multi-layered solid element: basics, patch simulation and its potential for thick composite structural analysis", 11th International LS-DYNA Users Conference, Dearborn, 2010