Safety Modeling of Lithium-ion Batteries under Mechanical Abuse

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Abstract

Lithium-ion batteries are one of the main energy storage devices in electrified vehicles. As their capacity and energy keep growing to meet the demand of longer driving range, their safety has become a primary concern due to their high energy and power density nature. Previously, abuse tests have been conducted to detect the failure conditions of lithium-ion batteries, but these tests can be expensive and time consuming. As such, computational modeling has played a more and more important role in evaluating battery responses under various abuse conditions. Here we present a multi-physical model for battery safety that is able to predict coupled mechanical, thermal, electrical and electrochemical responses of batteries using LS-DYNA®. In this framework, electrochemical behaviors of batteries are described by a spatially distributed equivalent circuit model, where polarization and damping effects can be captured by a resistance-capacitance network. While this framework can be applied to various abuse scenarios, we focus on its application in mechanical abuse in this presentation due to space limit. During mechanical abuse, the mechanical solver predicts the onset of internal or external short circuit at the initial stage, and then the coupled thermal, electrical and electrochemical solver captures the evolution of temperature and current distribution after short circuit initiation. To improve computational efficiency and allow the proposed model to be extended to module or pack level simulations, new element formulation and approximation approach developed recently are evaluated. Case studies show that using the new element type and approach may achieve comparable results while reducing computational time significantly. Details in model set up, parameters evaluation, and examples that show model capabilities will be presented. The future development of this framework and its experimental validation will also be discussed.

1-Introduction

Safety is one of the most important design factors of battery systems in electrified vehicles due to their high energy and power density nature. Abuse tests (such as impact or over-charge tests) are widely used to check the battery safety, but they are usually expensive, time-consuming and may not provide details of battery failure. Computational modeling, on the other hand, has become an important tool to evaluate the behaviors of batteries under extreme conditions because it is more cost-effective and efficient. In battery safety simulations, battery behaviors such as voltage, current density, temperature and their dependence on material properties and design factors can be captured, which can accelerate battery design and optimization process significantly. One challenge of battery safety modeling is that in a typical battery failure process, multiple physical fields (such as mechanical deformation, electrochemical response, heat dissipation, etc.) are involved and should be all taken into account. Most of previous battery models only focus on either mechanical behaviors [1] or electrical and thermal responses [2-3]. Another challenge is the computational intensity in large-scale simulations. A battery pack in an electrified vehicle may contains hundreds of cells and each cell usually consists of more than a hundred individual layers with distinguished properties. Resolving each layer in a pack or module level simulation can be very computationally intensive and expensive.

To build a computational tool for battery safety that covers relevant physical fields and is applicable to battery modules and packs used in actual vehicles, Ford and LSTC are collaborating to develop new keywords and solver capabilities for battery abuse responses in LS-DYNA. The framework and mathematical formulations of this tool and its application in various failure scenarios of battery cells can be found in Refs. [4-5]. In this paper, we briefly introduce recent progresses made in model development and solver capabilities. In particular, we focus on new element formulations and approaches that are able to accelerate battery simulations, which is

critical to extend simulations from cell level to module and pack level. The advantages and limitations of different element formulations and approaches are evaluated. Future development in model and solver is also discussed.

2-Model Development

2-1 Physical models

Our computational tool captures mechanical, electrical, electrochemical and thermal responses of batteries during their failure processes. As such, the developed battery safety models are multi-physics in nature and couple multiple solvers (mechanical, EM and thermal solvers) in LS-DYNA. The mechanical solver solves momentum conservation equations for displacement fields, which has the capability to deal with highly nonlinear transient dynamics with various contact algorithms. The electrochemical responses of a battery cell are captured by the Randles circuit model [6]. This model describes battery behaviors using a combination of circuit components shown in **Fig. 1**.

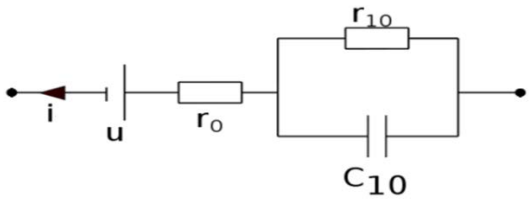

Figure 1: The Randles circuit model used in the EM solver. The meanings of i, u, r0, r10 and c10 can be found in text.

The potential difference between two end nodes in **Fig. 1** is calculated by $u - ir_0 - v_c$, where u is the local open-circuit voltage, i is the local transverse current density, r_0 is the local instantaneous resistance, and v_c is the local diffusion potential, which is the voltage across the resistance-capacitor pair and can be obtained from

$$\frac{dv_c}{dt} = \frac{i}{c_{10}} - \frac{v_c}{r_{10}c_{10}} \quad (1)$$

where r_{10} and c_{10} are resistance and capacitance in the resistance-capacitor pair. In order to improve the accuracy of the Randles circuit model, the parameters such as u, r_0, r_{10} and c_{10} are not constants. Instead, they are functions of state of charge (SOC), temperature and current direction. Because of that, the Randles circuit model can represent battery behaviors in a wide range of conditions. In addition, it is suitable for large-scale simulations due to its computational efficiency. In the EM solver, a Randles circuit connects two nodes in a pair of opposite current collectors to describe local unit-cell behaviors, and the entire cell is represented by a system of distributed Randles circuits. The electrical potential and current density in current collectors are obtained by solving the charge balance equation with the transverse current density given by the Randles circuit model. In the thermal solver, the energy conservation equation is solved to get the temperature distribution in 3D, where the heat source terms include Joule heating, reversible and irreversible heat generations. The calculated temperature is then used to update material properties in the mechanical and EM solvers.

2-2 Evaluation of material parameters

Depending on the types of solvers involved, different types of material properties are required to build a battery safety model. For the mechanical solver, we need to choose appropriate material models for different battery components and input the corresponding properties such as density, elastic modulus, and stress-strain relationship. MAT_PIECEWISE_LINEAR_PLASTICITY (MAT_024) is widely used to describe mechanical

properties of metals and can be used for current collectors. MAT_CRUSHABLE_FORM (MAT_063) can be used for electrodes due to their compressibility. The thermal properties such as thermal conductivities and heat capacities of battery components can be obtained from thermal measurements [7]. Since individual layers inside of a cell are thin, we may treat the entire cell as a body with uniform thermal properties for the sake of simplification. The electrical properties such as electrical conductivities of current collectors are usually well-known and therefore can be taken from the literature. On the other hand, the electrochemical properties of cells (i.e., parameters used in Randles circuit models) strongly depend on the cell chemistry and design, and should be measured by a set of well-designed experiments. The details of determining Randles circuit parameters as a function of SOC, temperature and current direction can be found in another paper [8] published in this proceeding. The general procedure is that we first measure voltage profiles of a cell from cycling tests under different conditions (e.g., different temperature, SOC, charge/discharge current). Then we use the Randles circuit model to predict the cell responses analytically. After that, we obtain the Randles circuit parameters by minimizing the difference between analytic solution and experimental measurement of voltage profile using optimization algorithms.

2-3 Approaches to accelerate battery simulations

As mentioned in the Introduction section, one of the main challenges in large-scale battery abuse simulations is the computational intensity since the size of a battery pack can be several orders of magnitude larger than the thickness of individual layers inside of a cell and resolving each layer in module or pack level simulations is expensive in computation. To make large-scale simulations more affordable, LSTC has developed a new element formulation called composite tshell element. It is one type of thick shell elements and one element can contain multiple layers of materials with different thicknesses and properties. PART_COMPOSITE_TSHELL is used to define a sequence of materials included in a composite tshell element, and its detailed usage can be found in Ref. [9]. Since one composite tshell element can contain multiple layers, it is suitable to model battery cells that consist of tens or hundreds of thin layers. Using composite tshell elements decreases the number of elements in a model significantly, which makes model development process more efficient. In addition, when resolving individual layers using standard solid/tshell elements, the thickness of elements is very small so that the time step used in the explicit scheme is highly constrained. On the other hand, with composite tshell elements the minimum element size increases considerably, which leads to a much larger time step and saves a lot of computational time in the mechanical solver. Initial results show that compared with using standard solid elements, using composite tshell elements can achieve almost the same results with much less time in different scenarios such as compression and shearing [10]. The EM and thermal solvers are also compatible with composite tshell elements. As such, the same mesh can be used in a model that couples different solvers, which simplifies pre- and post-processing work. The EM and thermal solvers usually employ the implicit scheme with large time steps. Moreover, when using composite tshell elements, they internally rebuild a solid mesh with all the successive layers and then create Randles circuits like that in standard solid/tshell elements [9]. Thus, the time saving in EM and thermal solvers when using composite tshell elements is minor. Fortunately, in some abuse scenarios such as impact, the mechanical solver takes the majority of the computational time, so saving time in the mechanical solver may reduce computational time of the entire model.

Along with composite tshell elements, LSTC has also developed meshless Randles circuit model to accelerate external short-circuit simulations. Here an external short-circuit means a short-circuit caused by contacts between bus bars in a battery module. In a traditional way, when simulating an external short-circuit in a module, we need to mesh all the layers in cells. With the meshless Randles circuit model, the cells themselves do not need to be meshed or even included. Instead, each pair of opposite bus bars is connected by one lumped Randles circuit (detailed settings can be found in the Case Studies section). In this way, the number of elements in a model decreases significantly, which saves tremendous computational time. One limitation of this approach

is that it assumes that each cell has homogeneous electrochemical properties, so it is mainly applicable to external short-circuit cases when cell deformation is minor and temperature in cells is almost uniform.

3-Case Studies

In this section, three examples of battery safety models are given. The first one shows the onset of an internal short-circuit and the subsequent evolution of voltage, SOC and temperature in a cell when impacted by a cylindrical object. This model uses standard tshell elements and demonstrates the capability of the developed tool to conduct multi-physics simulations of batteries under mechanical abuse. The second example shows an application of composite tshell elements in EM and thermal solvers, which is an extension to Ref. [10] where applications of composite tshell elements in the mechanical solver are given. The last example shows how to use meshless Randles circuit model in the case of an external short circuit.

3-1 Internal short-circuit simulations with standard tshell elements

The model settings of a pouch cell impacted by a cylinder object from its top surface is given by **Fig. 2**. Here the cell consists of 32 unit cells, and each unit cell contains positive and negative current collectors, cathode, anode and separator. Each component layer is meshed by standard tshell elements. MAT_024 is used for current collectors and separator, and MAT_063 is used for anode and cathode. The electrochemical properties of the cell are input to the model using the keyword EM_BATTERY_RANDLES developed recently. This keyword allows us to input Randles circuit parameters as a function of temperature, SOC and current direction for the entire cell (rather than unit cells). During the simulation, the cell bottom is fixed and the cylinder moves towards the cell with a constant speed. During the first 0.5ms, the structural equations are solved using equations from every solver. The mechanical deformation is assumed to occur at 0.5ms. After 0.5ms, all parts are set to be rigid and only electrical, electrochemical and thermal responses are updated until the end of simulations. The short-circuit is assumed to occur when the distance between current collectors is reduced by 10% of its original value. In that case the Randles circuit is replaced by a constant resistance (i.e., short-circuit resistance). Note that the short-circuit condition used here is for demonstration of model capability only. The actual condition is dependent on cell chemistry and design, which can be usually determined by comparing model results with controlled internal short-circuit tests. More general short-circuit conditions can be set using EM_RANDLE_SHORT.

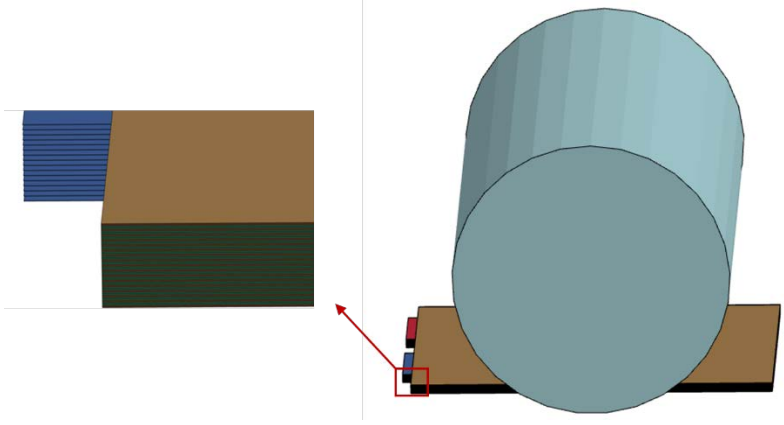

Figure 2: Geometry of a cell and a cylinder in the cell impact simulation.

The evolution of cell voltage and SOC during and after an impact is shown in **Fig. 3**. It can be seen that the cell gets shorted within 0.5ms. After the onset of the short, cell voltage and SOC drop instantaneously. After that,

the voltage and SOC decrease gradually depending on the discharge rate. During this period, current density changes according to the Randles circuit model, and temperature changes due to Joule heating. The distribution of current density and temperature at different time is displayed in **Figs. 4-5**, which clearly shows that the shorted area has high current density and temperature. The simulation results demonstrate that the developed tool is able to capture essential responses of a cell during an internal short-circuit event.

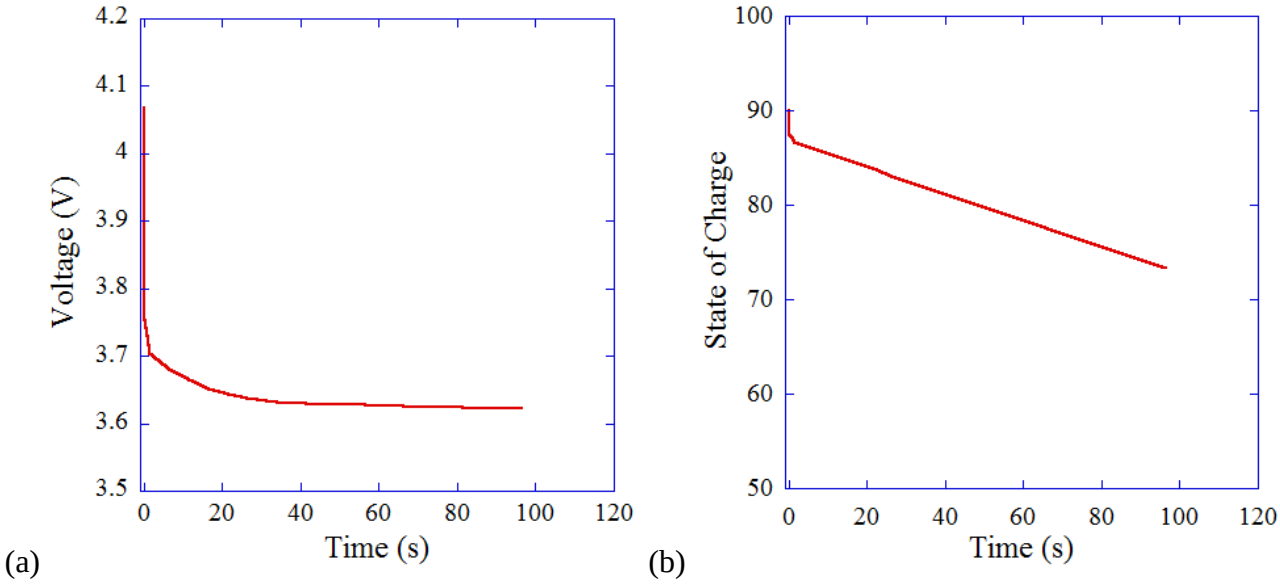

Figure 3: Evolution of (a) cell voltage and (b) SOC during the cell impact simulation.

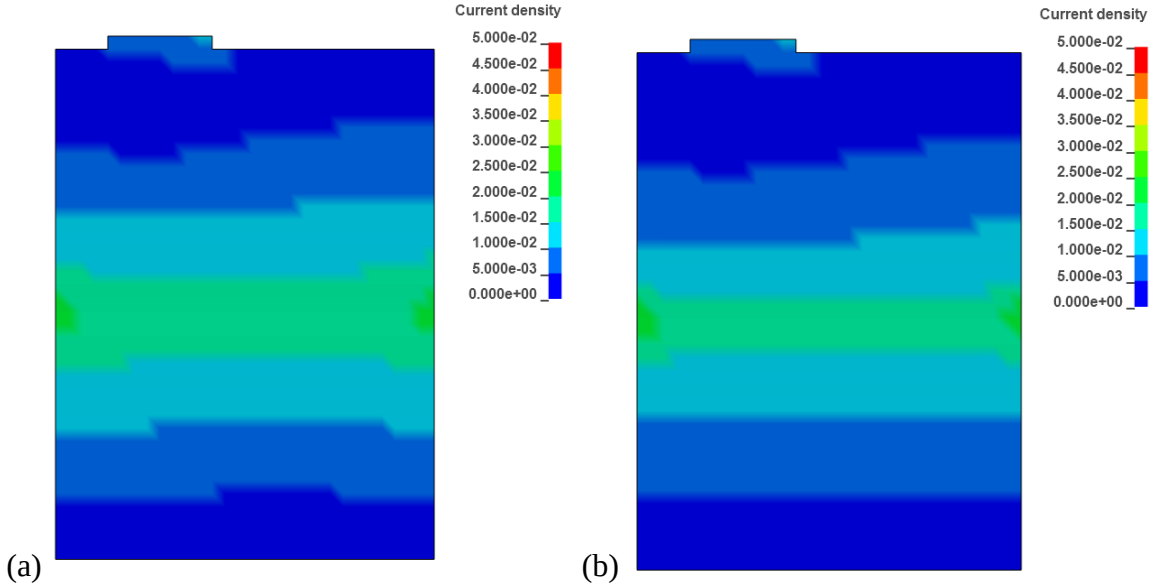

Figure 4: Distribution of current density at time (a) 6s and (b) 36s in the cell impact simulation.

3-2 Internal short-circuit simulations with composite tshell elements

In order to test the performance of composite tshell elements in EM and thermal solvers, we built two models with the same settings except that one uses standard solid elements and the other uses composite tshell elements, see **Fig. 6**. In the former, we resolve each layer in a cell and there are more than 100 layers/elements in the thickness direction. In contrast, in the latter there is only one (composite tshell) element in the thickness

direction. The thickness of a composite tshell element is the same as the sum of thickness of all layers that consist of a cell, so the geometries in both models represent the actual size of a cell. The main purpose of this exercise is to check if composite tshell elements can achieve the same results as standard solid elements, and the experimental validation of model predictions will be conducted in future. The keywords used in these two models are almost the same. The main difference is that in the model with composite tshell elements, cell parts are defined by PART_COMPOSITE_TSHELL instead of PART, and the Randles circuit parameters are input through EM_RANDLE_LAYERED instead of EM_BATTERY_RANDLES. In the simulations, the central part of the cell is assumed to have high resistance at the beginning, and then the resistance drops to a small value after 5 seconds, which mimics the event of internal short-circuit without involving mechanical deformation. In the other regions, opposite current collectors are connected by distributed Randles circuits with properties depending on temperature, SOC and current direction.

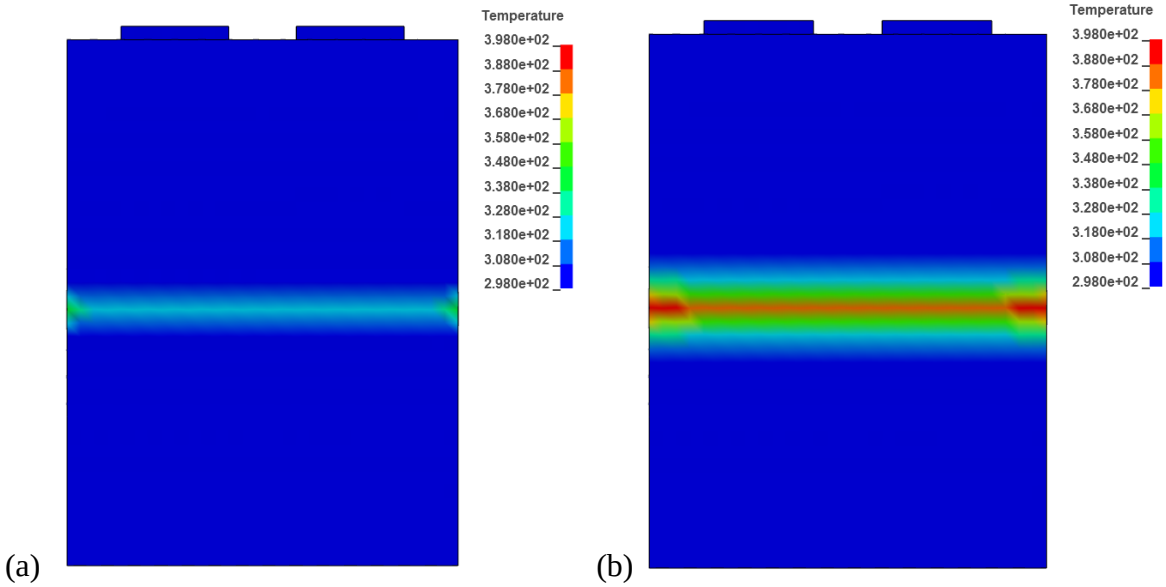

Figure 5: Distribution of temperature at time (a) 6s and (b) 36s in the cell impact simulation.

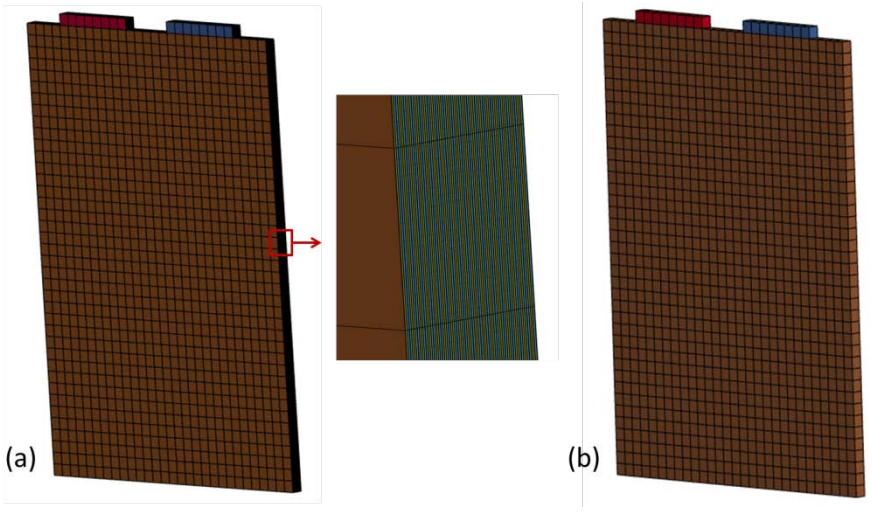

Figure 6: Two models with the same settings except that the cell is meshed by (a) standard solid elements and (b) composite tshell elements.

The comparison of voltage evolution, distribution of current density and temperature are shown in **Figs. 7-9**. It can be seen that when the resistance in the cell center drops after 5 second, the voltage drops to a small value immediately. In the meanwhile, current density in the central region increases due to short-circuit, and then temperature in that area increases rapidly. The temperature in the other regions of the cell increases gradually due to the thermal conductivity. All these observations are consistent with what we expect.

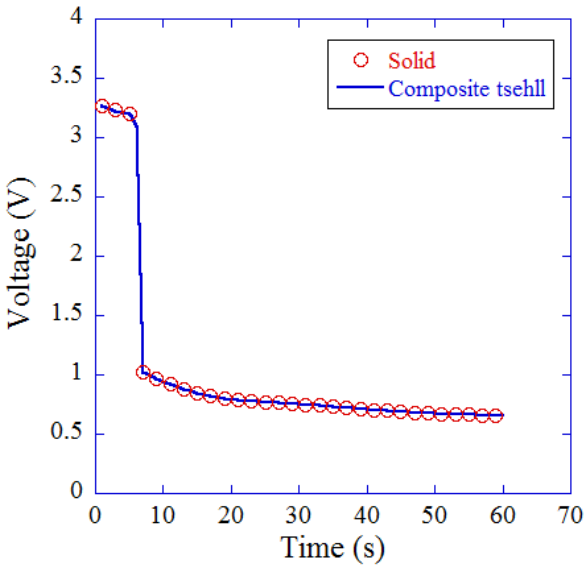

Figure 7: Comparison of voltage evolution in a cell from two models with different element types.

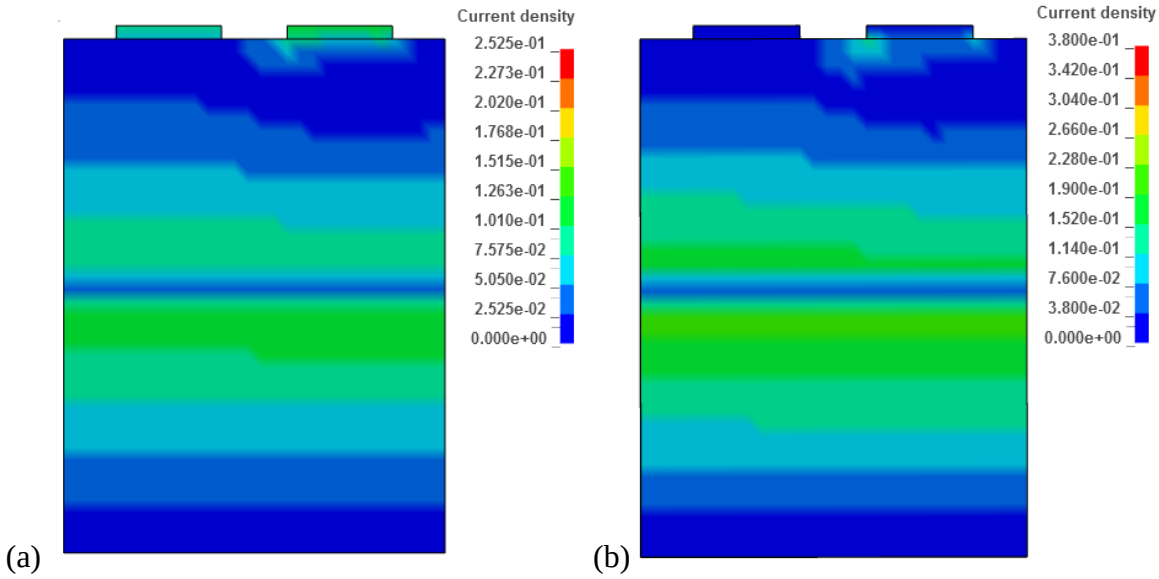

Figure 8: Comparison of in-plane current distribution at time 10s in a cell from models using (a) standard solid elements and (b) composite tshell elements.

One may find that **Fig. 8a** and **Fig. 8b** use different color scales. For composite tshell elements, the post-processing tool LS-PrePost® does indeed not visualize the transverse current density but the in-plane current density averaged over all the positive current collectors in composite tshell elements. As such, **Fig. 8** shows in-plane current densities from two models for the sake of the comparison. Note that **Fig. 8a** shows the current density in a current collector while **Fig. 8b** shows the average current density. Their magnitudes are not

supposed to compare directly, so we use different color scales in these two figures. It is emphasized here that although current densities of individual layers in composite tshell elements cannot be visualized, they are stored in the EM solver internally and moreover, they are very close to the current densities of current collectors in the model with standard solid elements, as can be seen in the temperature distribution comparison (**Fig. 9**). One may also find that the current density shown in **Fig. 8** has smaller values at the shorted area. It is because a short-circuit leads to a large transverse current density at the shorted area, and then the in-plane current density at this area is smaller than the one in the surrounding areas due to current conservation. Although both in-plane and transverse current densities contribute to the heat source terms, the latter dominates the heat contribution because of its larger magnitude. Thus, at the shorted area, the temperature is high even though the in-plane current density is low.

Figs. 7-9 also demonstrate that the voltage, current density and temperature obtained from the two models are almost identical and thus composite tshell elements could replace standard solid elements in EM and thermal solvers. The advantage is the lower number of elements when using a composite tshell elements model. When we build a battery safety model that couples mechanical, EM and thermal solvers, we use the same mesh for all the solvers making the model pre-processing more convenient.

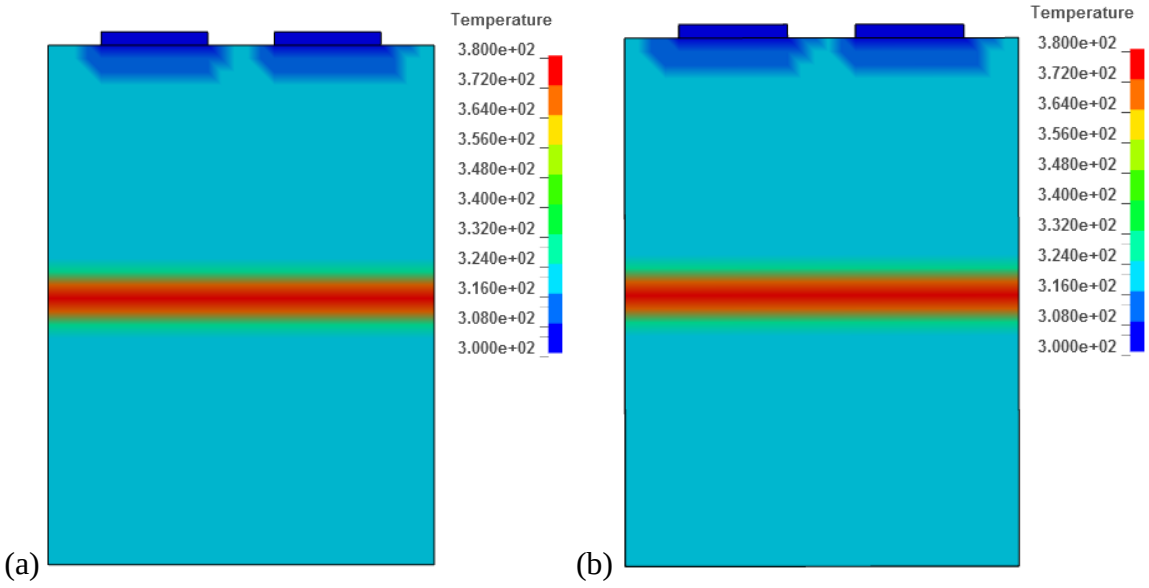

Figure 9: Comparison of temperature distribution at time 10s in a cell from models using (a) standard solid elements and (b) composite tshell elements.

3-3 External short-circuit simulations using the meshless Randles circuit model

The main purpose of this study case is to show an application of the meshless Randles circuit model. Here a 5P4S module is impacted by its cover from the top (see the impact direction in **Fig. 10a**). The deformation of bus bars may cause contact between opposite bus bars leading to an external short-circuit. As mentioned previously, for module level simulations, we generally need to mesh all the cells. The simulations may then take a long time. In some scenarios, like the example shown below, the cells themselves are not expected to be largely deformed and do not constitute an area of interest. In this case we may accelerate simulations using the meshless Randles circuit model, where the cells do not need to be included (see **Fig. 10a**). Each pair of opposite bus bars are connected by a single lumped Randles circuit (see **Fig. 10b**). To activate the meshless Randles

circuit model, we use EM_RANDLE_MESHLESS instead of EM_BATTERY_RANDLES to input the Randles circuit parameters, and set CONTYPE as 5 in EM_ISOPOTENTIAL_CONNECT to connect two bus bars.

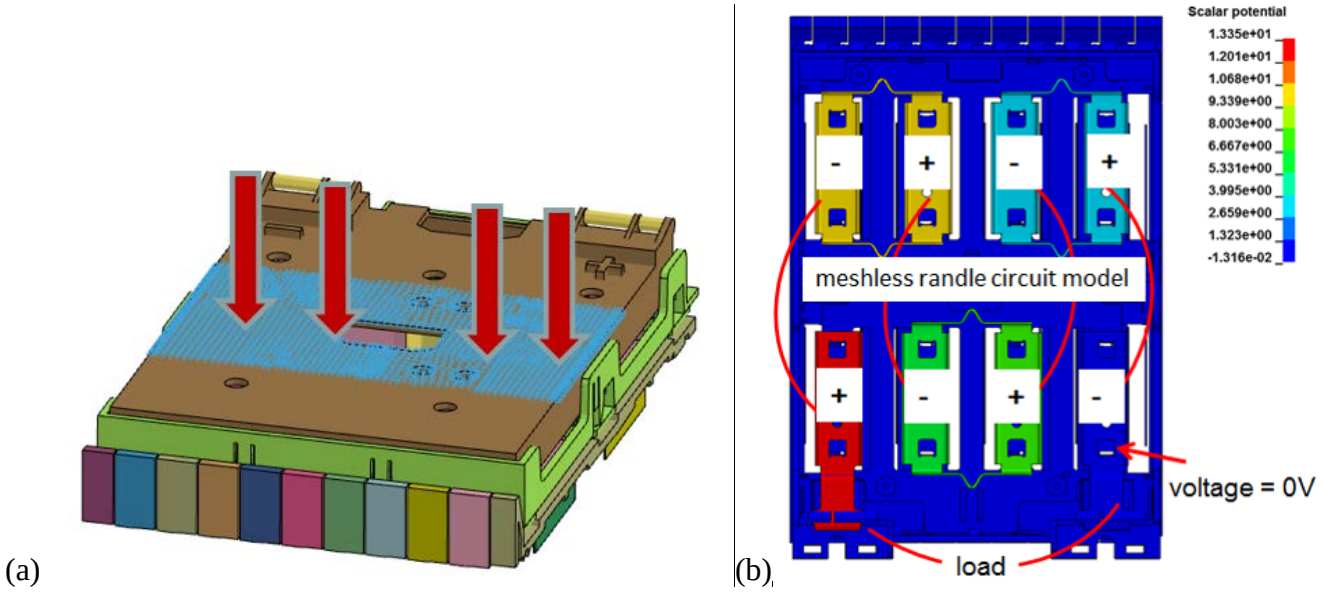

Figure 10: (a) Settings of a module impact simulation using the meshless Randles circuit model where cells are not included; (b) Pairs of opposite bus bars are connected by lumped Randles circuits in the meshless Randles circuit model.

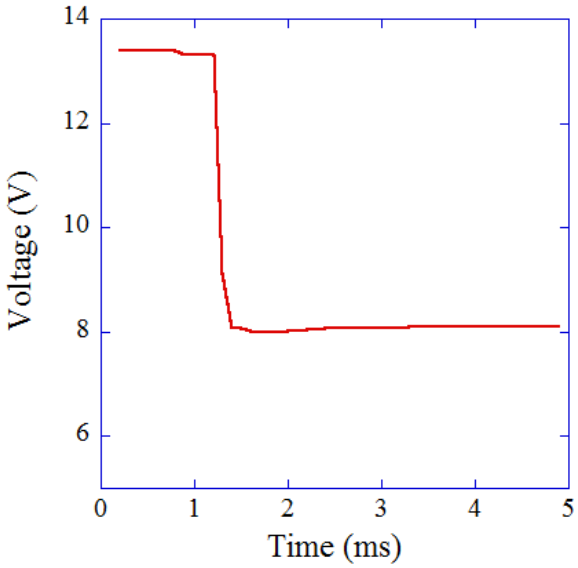

Figure 11: Module voltage evolution in the module impact simulation.

The voltage evolution, distribution of current density and temperature at different time are shown in **Figs. 11-13**. It can be seen that when the top cover moves down, bus bars start to deform. When opposite bus bars touch each other, an external short-circuit occurs and causes a sharp drop in module voltage. After that, the current density in shorted area increases rapidly together with the temperature. It is noted that a large current density is found in shorted bus bars and the bus bars connected to the shorted ones through the lumped Randles circuits. It

is because these bus bars form a loop after the onset of external short-circuit, and the large current induced by short-circuit flows through the entire loop rather than the shorted area alone. These simulation results show that voltage, current density and temperature in an external short-circuit event can all be captured using the meshless Randles circuit model, which has a potential to save a large amount of computational time.

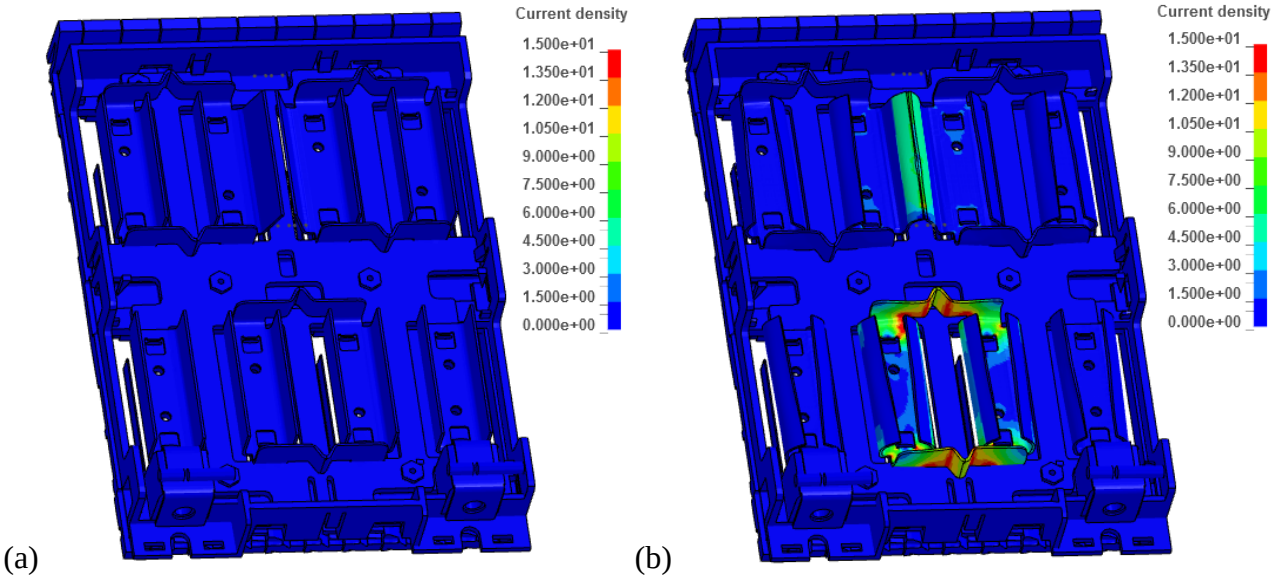

Figure 12: The current density distribution at time (a) 0ms and (b) 4ms in the module impact simulation.

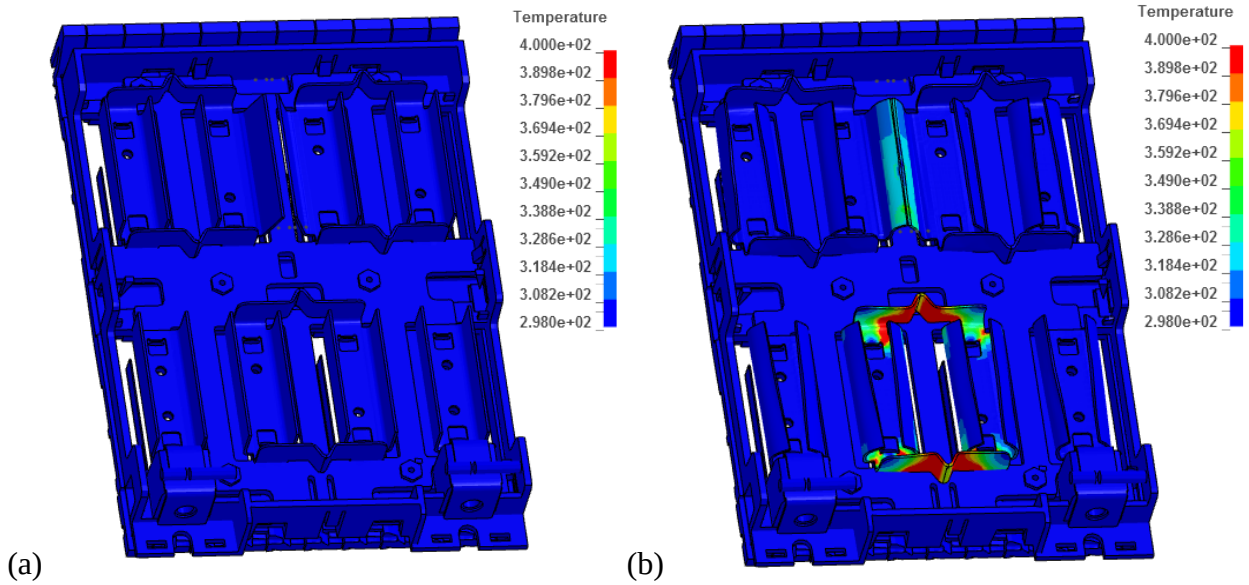

Figure 13: The temperature distribution at time (a) 0ms and (b) 4ms in the module impact simulation.

4-Conclusions

A computational tool that couples mechanical, EM and thermal solvers in LS-DYNA has been used to capture the responses of battery cells and modules under various mechanical abuse scenarios. To reduce computational time in large-scale simulations, composite tshell elements and meshless Randles circuit model have been developed. The former is suitable to the cases where properties of individual components in cells are relevant such as an internal short-circuit event. Initial results show that mechanical, EM and thermal solvers are all compatible to composite tshell elements. Compared with standard solid/tshell elements, using composite tshell elements may get almost the same results and save time in the mechanical solver significantly. The latter works for the cases where the cell properties are uniform and the area of interest is outside of a cell such as an external short-circuit caused by contact of bus bars. Since cells do not need to be included in the meshless Randles circuit model, the number of elements and therefore the computational time reduces considerably. Work is underway to test the performance of composite tshell elements in models that involve all three (mechanical, EM and thermal) solvers. Future work will focus on calibrating model parameters and validating model predictions by abuse tests.

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