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**Assessing battery safety using a combined simulation
approach from cell to vehicle level**

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Executive Summary

Assessing a Li-Ion battery in terms of safety and reliability requires a detailed understanding on cell level on the one hand, and a full understanding on system level on the other hand. Only in this way, one can extract accurate loads acting on the cell which are caused on vehicle level. The virtual assessment of cell safety in crash and misuse cases requires the global simulation of crash scenarios including the influence of State-of-Charge (SoC) and State-of-Health (SoH) and the corresponding impact on cell level. In a detailed view on cell level, this paper investigates the mechanical deformations of the cell and the potential risk of a following thermal runaway and its thermal propagation to neighboring cells or modules.

For simulating a realistic behavior on large scale models like bottom floor batteries in battery electric vehicles (BEV), a proper method for model reduction is essential. In this paper an approach is presented in which various scale models are combined for substituting single components in each model scale by representative models which allows fast calculation times on the one hand, and an accurate global behavior on the other side. Following this approach, it is possible simulating vehicle crash scenarios and assessing the impact on the cell-inner electrode layer structure.

1 Introduction

There are diverse challenges being placed on a battery design in order to maintain the acceptance of battery-electric vehicles (BEVs). These vary from a minimum required range, via an optimized battery lifetime that still guarantees this range even after many years of use and after hundreds of thousands of kilometers driven, up to reduced costs to be able to sell the vehicle at an attractive price. However, over all of these challenges, there is one overarching requirement that must consider all of the previously mentioned points and is an absolute must for battery construction: safety.

One of the goals in high voltage traction batteries (HV batteries) based on Lithium-ion technology is the prevention of electrical short-circuits in the high voltage system, even after severe distortion for example after an accident. Another goal is the protection of the Li-ion cells in the HV battery from heat, penetration by sharp

objects or severe mechanical loading. If the previously mentioned challenge of customer acceptance is to be met, a safe battery design is required that is low-cost, lightweight and optimally cooled.

In view of short development times and the continuously changing challenges, the development of safe battery constructions requires the use of simulation in early development stages so that the identification of any necessary stiffening and build space for mechanical integrity is possible in the conceptual phases.

If the battery design is to be evaluated regarding possibly safety-relevant load cases, then adequate and accurate modelling, above all of safety-critical components, is required. This includes not only the prediction of electrical short-circuits through the modelling of the HV system or the prediction of possible cooling system leakage, but above all the improved understanding of the Li-ion cell from a safety-relevant point of view.

A methodology will be presented that estimates the safety of the entire battery starting with the deformation and damage of a single cell. In this approach single components like cells, HV wires or EE parts are tested and evaluated in terms of stiffness and their contribution to the overall stiffness. Then the single components are simplified in the global model for ensuring an accurate global mechanical behavior. With that global behavior, relevant loads are derived for the single components which are then simulated more in detail. In a further step, the damage of the single component like an individual Li-ion cell is assessed using typical load cases (crash, crush, nail penetration). In a second step, the consequence of the event on cell safety is determined, i.e. whether thermal runaway in the cell is imminent or not. A third step assesses whether the overheating of an individual cell will lead to a system-wide thermal runaway of the HV battery and if yes, how fast this process will propagate. Figure 1 shows the generic workflow for such an approach.

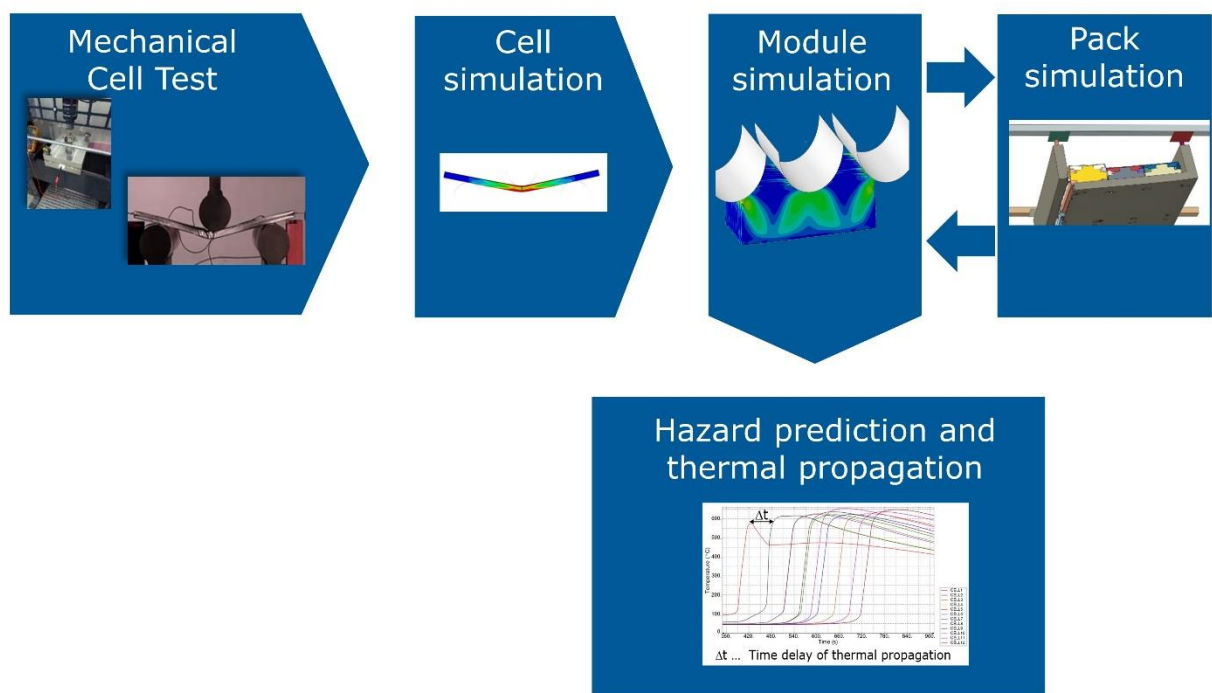


Figure 1: schematic workflow diagram for Li-Ion cell safety assessment in vehicle crash conditions

2 Thermal runaway at its root causes

The growth of the Li-ion batteries market during the last 30 years owe its trend to the efficiency and safety of this technology to store electrical energy. The idea to store energy and use it when needed is a common concept of the modern industry and the Li-ion batteries provided an efficient and compact solution for many portable device applications. Under particular stress conditions, the stored energy could be released, mainly in form of heat, even if not needed and not requested by the user: this phenomenon, that can be even dangerous in some cases, goes under the name of “Thermal Runaway”. Due to the variety of materials inside the Li-ion Battery, the reactions due to the thermal runaway are complex and difficult to describe. Some compounds inside the Battery are even difficult to identify like to Solid Electrolyte Interface, so the reactions list inside the battery it is difficult to predict.

Summarizing, a thermal runaway can be triggered by different stress conditions types:

- Mechanical stress: Structural load can produce a deformation of the Battery layers and lead to the rupture of the separator, as consequence there could be an internal short circuit and fast energy release.
- Nail penetration: An external object is introduced in the battery volume causing the rupture of several layers. The material constituting the object determine the entity of the short circuit and the consequent exothermal reaction.
- Thermal stress: Thermal stress, if it is enough to lead the cell temperature to a threshold value, it can starts a list of reactions that take part usually in a sequential order. Each reaction is triggered by its own threshold temperature that can be reached by the heat generated by the previous reaction.

Modeling

In general, the approach for the modelling of physical phenomena can be analytical or empiric. For the case of Thermal Runaway, the analytical approach it's really complex due to the variety of materials inside the cell and the high number of variable to which the exothermal reactions are dependent from.

The approach proposed is empirical, the aim is to map the exothermal reactions of a Li-ion cell during the Thermal Runaway as a function of temperature. The final goal is to reproduce such exothermal reaction in FEM simulations.

For modeling the behavior of cells in thermal runaway a 2-step-approach was chosen which combines information determined in physical tests with an analytical fitting of mathematical functions which are based on electro-chemical background knowhow.

1. Accelerating Rate Calorimetry Test

The test is conducted pushing the Li-ion cell temperature to the threshold temperature inside an adiabatic environment (ARC bomb). Once the cell will start to generate heat, the sensors positioned inside the bomb will monitor the temperature and pressure increasing.

The Arrhenius law states that the reaction rate of a reaction depends by the temperature of the reactants. With this basis, the mapping of the exothermal reaction of the Li-ion cell can be reasonably expressed by a function that express the heat power released with temperature dependence.

2. Heat power function determination

The observation of several experiment of Thermal Runway in ARC bomb lead to the conclusion that is possible to model the majority of these events with the same mathematical functions. These mathematical functions have been deducted by complex fitting curve algorithms.

3 From small scale to big scale: From cell to battery pack level including vehicle structure

From a simplified point of view, a Li-ion cell consists of a thin layers of metallic electrodes coated with the corresponding active material (graphite or Li-metal oxide) that are usually electrically isolated by a plastic (polyolefin) separator and connected with ion-transporting liquid or gel electrolyte. These layers are only several tens of micrometres thick and their mechanical attributes are dependent on the charging state of the cell. To accurately model this complex structure, a special method to characterise the cell attributes has been developed. On the one hand, special tests and automated parameter identification tests determine the mechanical behaviour of the cells. On the other, the test results are used to derive when internal short-circuits and thermal runaway could occur. A thermal runaway is a self-amplifying, exothermic chemical process in which the cell produces heat and generally leads to a fire in the individual cell.

The method is adapted in such a way that the cells can be integrated using replacement models in battery modules and battery systems. This has the advantage that the influence of mechanical behaviour of the individual cell in the network of the total system can be evaluated. Figure 2 shows the comparison between test and simulation results for 3 point bending test on cell level.

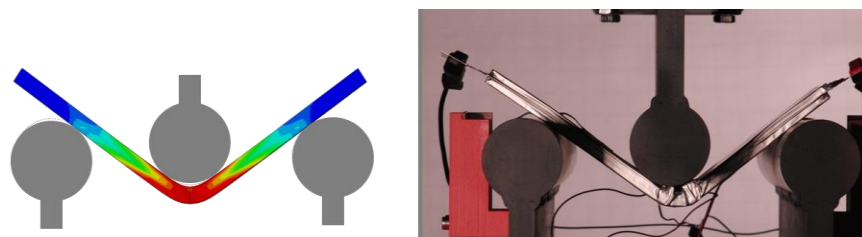


Figure 2: 3 point bending test on cell level: correlation between test and simulation results

In the next step, the battery cell replacement models are derived. These models are intended for use on a battery module and pack level.

The challenge for the simulation of the replacement models is guaranteeing the high significance and accuracy in the simulation results on module and pack levels and simultaneously keeping the finite element model (FE) calculation time sufficiently low

For assessing the battery pack itself, the mounting to the vehicle and its structural reinforcements has to be considered. Only in combination of vehicle stiffness and battery pack stiffness including cells, modules and electric current carrying parts a total system view can be ensured with an optimized global packaging concept. Simulating the global behaviour now, leads to the loads and deformations which occur on small scale model level, down to single cell level. With these boundary conditions from global load case, the single cell is simulated and the damage predicted.

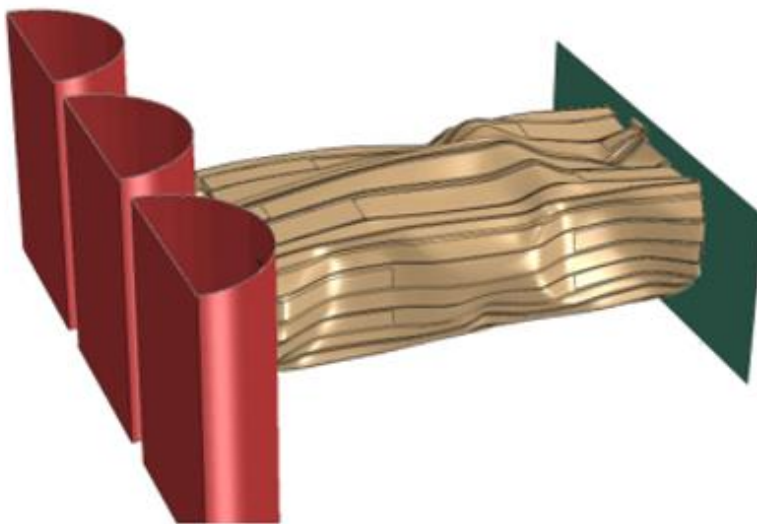


Figure 3: module crush test simulation

Figure 3 shows a typical load case in which the module is compressed to 50% of its original length. They should be no safety-relevant effect such as a fire or an explosion. The load case described is intended to clearly demonstrate how high the development effort for the construction of a module is to withstand this load case and also to show how stringent the requirements on the simulation model are in order to be able to evaluate this development target. Deformations of this magnitude require that all relevant components have representative models that are able to predict and consider damage to the component. This entails the FE simulation calculating a damage factor per element; if the factor's limit is exceeded then the material damage is calculated that has significant influence on the further course of the simulation. The quality of the material modelling also affects

the quality of the global simulation results. Diagram 3 shows such a simulation where a battery pack component failure is calculated.

Hence the prediction of global deformation on a module and pack level in crush and crash load cases is possible using damage models and mechanical characterisation of the cells. On a cell level, the results are an evaluation regarding possible short-circuits and safety in damage events.

Figure 3 shows the integral contribution of the Li-ion cells to the total stiffness of the modules. A correct deformation of the modules cannot be calculated without considering the corresponding material attributes of the cells (stiffness, elongation at rupture, etc.). This emphasizes once more the significance of the accurate modelling of the cell itself.

Integration of Modules in Pack Simulation

Up to forty such modules are incorporated in a battery pack in a modern BEV with a range of several hundred kilometres. In order to be able to represent such a battery pack in an FE model, the individual module models need to be simplified and yet remain sufficiently accurate to permit the realistic simulation and evaluation of the total battery pack stiffness. This is the particular challenge of model reduction. If the model is neglected in the pack simulation then this may lead to an oversizing of the battery housing.

Figure 4 shows a side pole crash test for a complete HV battery. The deformation of the battery frame can be clearly seen, which leads to contact between the frame and the modules. In order to determine whether this contact has safety-relevant consequences, the model deformations are transferred to the detailed module FE model and damage is predicted on a cell level.

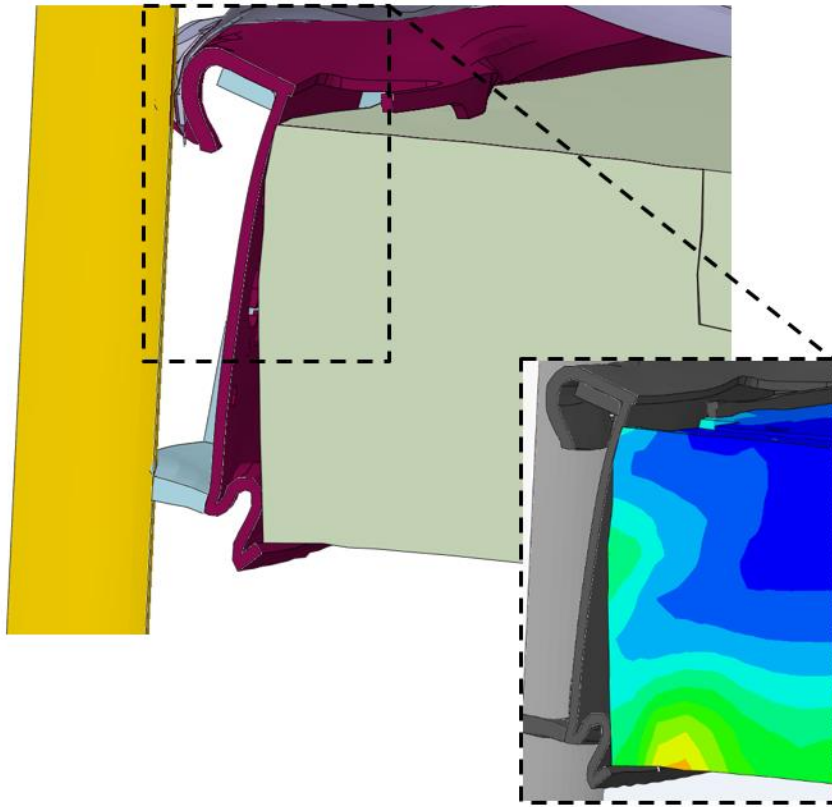


Figure 4 side impact of vehicle and its impacts on pack and module level

4 Hazard prediction

The previous section describing the modelling of Li-ion cells concentrated primarily on the representation of the mechanical behaviour of cells on a cell, module or pack level. This permits the exact simulation of the global mechanical behaviour of a battery. If the battery design is to be evaluated regarding safety, a criterion for the safety-relevant evaluation of cell deformation needs to be defined.

Generally speaking, the severe deformation of a cell or the penetration of an external object into the cell leads to damage of the separator layers in the cell, which in turn lead to a cell-internal short-circuit between the cathode and anode. The consequences can be gas leakage, formation of thick smoke and even cell combustion. In the case of fire, it is possible that thermal runaway of the whole battery occurs.

AVL has developed a method that is able to describe the temperature development during thermal runaway for a cell. The method involves creating a tool that takes the calculated deformations from the pack simulation and the derived cell behaviour from the previously mentioned tests. This permits the simulation of hazard cases on a cell level and subsequently evaluating constructive measures to thermally isolate burning cells.

The AVL methodology also enables an important question to be answered: What happens if, for whatever reason, one of the cells begins to combust? This could be because of an internal cell failure (perhaps due to contamination or dendrite formation), or due to external influences such as overcharging, penetration of sharp objects, short-

circuit of the pole, severe deformation or overheating. Is it possible to prevent the thermal propagation of thermal runaway to neighbouring cells in such a case? Or is it possible, by using suitable measures, for example thermal isolation or cooling, to delay thermal propagation to enable the vehicle to be brought to a standstill and allow the passengers to evacuate?

The simulation of thermal runaway of an individual cell and the propagation to neighbouring cells to the activation point of the neighbouring cells, and hence the calculation of the time delay between the thermal runaway of the first and subsequent cells is made possible by the implementation of the physical and chemical laws governing heat release based on measurement data, cell chemistry characteristics and several other physical attributes. Diagram 5 shows the simulation results for a typical BEV module. It can be seen that without special measures, thermal runaway in neighbouring cells occurs within 30-45 s. This correlates well with practical experience from corresponding real safety tests. The simulation results provide the basis in battery development for a comparison of different safety strategies such as thermal isolation, optimised cooling possibilities or heat removal. Thus the urgent question asked above can be answered using the simulation results and finally reliable and above all safe HV batteries can be developed.

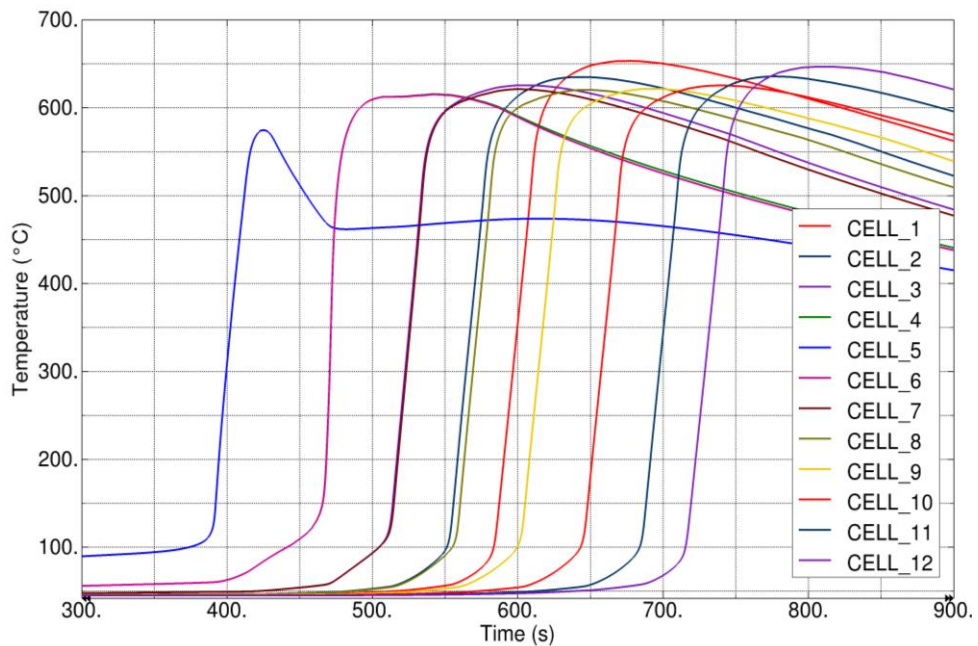


Figure5: Simulation of thermal propagation behaviour in a BEV module

Figure 5 shows the simulation results for a typical BEV module. It can be seen that without special measures, thermal runaway in neighbouring cells occurs within 30-45 s. This correlates well with practical experience from corresponding real safety tests. The simulation results provide the basis in battery development for a comparison of different safety strategies such as thermal isolation, optimised cooling possibilities or heat removal. Thus the urgent question asked above can be answered using the simulation results and finally reliable and above all safe HV batteries can be developed.

5 Summary

The simulation and subsequent evaluation of safety-relevant load cases on HV battery systems is a challenge for all participating disciplines in general and all areas of FE modelling specifically: Large models with many contacts and a range of materials from metal to plastic to foam, rubber or resins. Since every component either contributes to structural integrity or to electrical safety, it is necessary to have damage models for almost all materials used. Modelling, material characterization and final evaluation according to the mechanical loading of Li-ion cells also pose huge challenges regarding battery simulation. The methodology described in this contribution (see also diagram 6) shows a path from the testing of mechanical characteristics of individual cells, via the stiffness and crash simulation on a module and pack level, up to a method for the evaluation of electrical short-circuits, hazard events on a cell level and the propagation of cell fire after thermal runaway to neighbouring cells and modules.

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