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## **Introducing an approach to predict the time-dependent mechanical, electrical and thermal behaviour of Li-ion batteries due to crash loads**

Simon F. Heindl<sup>1</sup>, Christoph Breitfuss<sup>1</sup>, Robert Greimel<sup>1</sup>, Wolfgang Sinz<sup>1</sup>,  
Christian Ellersdorfer<sup>1</sup>, Florian Feist<sup>1</sup>, Clemens Fink<sup>2</sup>

<sup>1</sup>*Vehicle Safety Institute, Graz University of Technology, Graz*

<sup>2</sup>*AVL List GmbH, Graz*

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### **Executive Summary**

Nowadays, lithium-ion batteries are the predominant energy storage technology for vehicles with electrified drive trains. In case of an accident mechanical loads on Li-ion cells may cause an internal short-circuit which can further lead to severe exothermic reactions (e.g. smoke, fire, explosion). Existing numerical methods to estimate the time-dependent mechanical, electrical and thermal processes are not sufficient at present. For that reason a novel approach has been developed. Three major parts - explicit non-linear structural analysis (FEA), implicit multi-physical simulation and an interface to link these two simulation tools - have been combined to form a continuous work-flow. While the FEA model has been set up using a microscopic scale mesh, the multi-physics code was extended by a short-circuit model. This approach is capable of predicting the cell behaviour due to crash loads (e.g. acceleration, deformation).

*Keywords: lithium battery, battery model, short circuit, simulation, safety*

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# 1 Motivation

Electrical energy storage systems (EESS) for electric vehicles (EV) and hybrid-electric vehicles (xHEV) are mainly based on lithium-ion technology. A significant disadvantage of these batteries is their tendency to exothermic reactions under certain conditions (e.g. mechanical deformation). In case of a vehicle crash indentation or penetration of Li-ion cells may lead to severe consequences for human health and for the environment. Mechanical load on the battery cell seems to be one of some possible worst-case scenarios for electrified vehicles. For instance this may cause damage to the separator layer and can further lead to an internal short-circuit. In general, discharge processes induce heat release within the cell domain due to e.g. internal ohmic resistances. Short-circuit events can be seen as a certain occurrence of cell discharge and consequentially show a significant higher rise in temperature. If the heat produced (e.g. short-circuit) exceeds the heat dissipated (e.g. battery cooling system) this may end up in an exothermic reaction commonly known as *thermal runaway*. Figure 1 shows a state-of-the-art automotive quality Li-ion cell's reaction when being punctured. Due to this inherent hazard potential of Li-ion cells, their protection is essential and numerical prediction methods are subject to research at the moment.

Normally a crash happens within a split second. Unfortunately chemical reactions triggered by mechanical damage inside a battery cell may evolve over a longer period of time. Undesirable effects may arise unnoticed and may lead to severe consequences hours later. A main challenge in the development of predictive numerical methods is the linking of these two time domains from milliseconds up to hours.



Figure 1: Puncture penetration test with pouch-type Li-ion cell.

# 2 State of the art

**Li-ion cell hazards** To ensure an acceptable standard of safety the intrinsic dangers of Li-ion cells have to be known well. Sinz [1] gave a comprehensive survey of battery hazards which can be summarized in the four groups as follows: chemical hazards, thermal hazards, electrical hazards and mechanical hazards. This study focuses on mechanical mistreatment of Li-ion cells which in turn may cause damage to the battery's separator and may further induce short-circuit events.

Yamaki [2] has depicted the relation of heat produced and heat dissipated. If the heat produced is predominant the system's getting unstable. This state is called thermal runaway. In the case of Li-ion cells a thermal runaway may initiate further chemical processes which can lead to decomposition of cell material, gas generation and may cause venting of reaction products. The following graph from Roth [3] gives an overview of potential Li-ion cell venting gas substances and their characteristics.

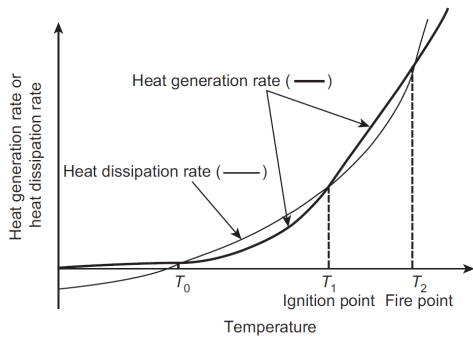


Figure 2: Heat generation rate vs. heat dissipation rate [2].

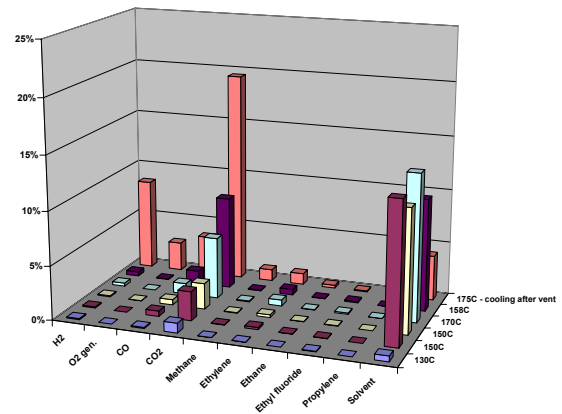


Figure 3: Concentration of substances released during Li-ion cell venting [3].

**Mechanical battery simulation** To predict the effects of mechanical load on a cell's components finite element analysis (FEA) methods are in use. Depending on the application one can choose from macroscopic (also: homogenised), microscopic (also: micro-scaled) or combined modeling approaches. Macroscopic models are characterized by rough discretisation and combination of multiple cell components to form summarized elements with average material properties. Microscopic models show a detailed representation of every part or layer inside the cell including precise geometry and material properties. Breitfuss [4] gave an overview on mechanical modeling approaches and showed an example for both macroscopic as well as microscopic simulation mesh concepts (see figures 4 and 5).

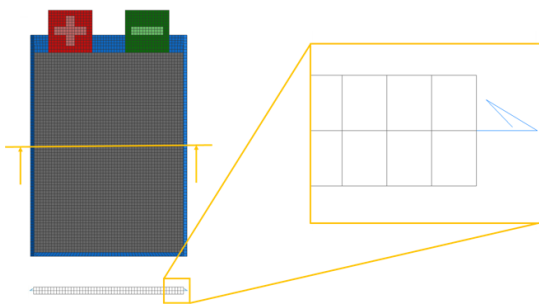


Figure 4: Macroscopic modeling approach [4].

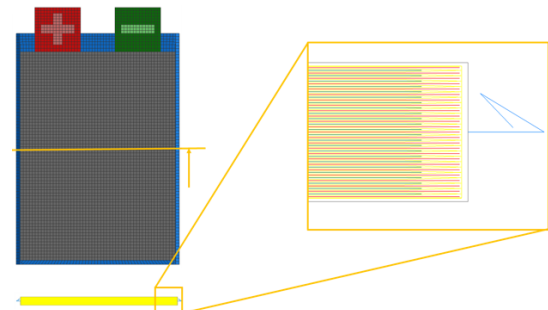


Figure 5: Microscopic modeling approach [4].

**Short-circuit detection (mechanical failure criteria)** A short-circuit may occur if the cell's separator is damaged. To detect short-circuit situations material failure criteria are applied on the cell model. For macroscopic models this is done by calculation of characteristic values for summarized elements called "Representative Volume Elements" (RVE). This characteristic mechanical parameter correlates geometric deformation (e.g. dilatation) of an RVE with a short-circuit of the cell and is determined by experiments. In literature [5, 6, 7, 8, 9, 10, 11, 12] followed this approach. For microscopic models a separator break is given by the material's strength and additional information about the electrical behavior of the material under mechanical load. Chen [13] and Matzer [14] used a ball shaped penetrator to correlate an applied force on a separator foil with a short circuit. Plaimer [15, 16] conducted experiments to examine the trade-off between mechanical and electrical properties of separator materials. A compre-

hensive state of the art for mechanical battery simulation and short-circuit detection has been written by Breiffuss [4].

**Multiphysical battery simulation and abuse simulation** Simple simulation approaches are based on equivalent electric circuits using so called "Randle's elements" (e.g. [17]). More complex models try to abstract the processes running inside the cell at different levels of abstraction. These multi-physical battery simulations are used to estimate the cell's present state (e.g. state of charge, state of health) as well as to predict the cell's response in case of a short-circuit. Electro-chemical simulations represent electrical and thermal processes as well as chemical reactions and energy balances of a cell on a high level of detail and require a certain amount of (experimental) validation work [18] [19] [20]. If more simple modeling approaches are requested electro-thermal models can be chosen. To simulate the behaviour of Li-ion cells (e.g. cell voltage, temperature evolution) up to some hours time these models are feasible [21][22]. For short-circuit simulations electro-thermal models need to be extended by a short-circuit model to reproduce the special processes during a short.

**Co-simulation of mechanical and electro-thermal simulation** By now, effects in different time regimes are not solved sufficiently by common numerical methods. Therefore simulation tools should, besides being universally applicable and user friendly, link the solvers for structural mechanics (FEA) and time-dependent (multi-physics) problems. The only known framework for combined battery simulation models for different tasks has been published by NREL [23].

### 3 Approach

**Innovation** Currently most published models for short-circuit detection are based on the RVE concept. Further known short-circuit simulations are designed for speciality applications and hereby are dependent of the certain situation (e.g. models for nail-penetration [24]). Current thermal models [25] using a source term for short-circuit heat release are less detailed and therefore not applicable to e.g. assess different separator products in terms of battery safety. The current paper demonstrates the prediction of the time-dependent mechanical, electrical and thermal behaviour of Li-ion batteries due to crash loads by combination of several sub-models as listed below:

- A finite element simulation, including a specially detailed separator model, allows precise prediction of the mechanical state of the cell's components without uncertainties caused by summarized material properties
- A geometry interface tool for the application of a mechanical separator failure criteria and for automatic mesh translation from FEA to the multi-physical simulation
- A short-circuit model as an add-on to a battery simulation software that calculates the electrical and 3-dimensional thermal response of a Li-ion cell due to arbitrary short-circuit situations

The basic principle behind this approach is outlined in fig. 6 and has been first described by Feist [26] in 2013.

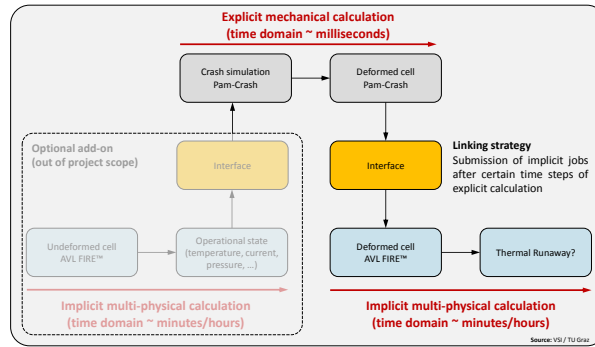


Figure 6: An approach to predict time-dependent effects in Li-ion cells due to crash loads

**Research question** To predict if a given mechanical load on a Li-ion cell is tolerable the central research question has to be answered:

*How to combine the different time regimes of explicit FEA and implicit multi-physical simulation into one coherent work-flow?*

This unfolds concrete development tasks listed as follows:

- Correlation of electrical and mechanical characteristics of separator materials
- Development of a detailed FEA model which can identify mechanical damage (e.g. separator layer failure) due to crash loads
- Understanding of cell internal processes preceding short-circuit events
- Development of a multi-physical model which can predict the 3-dimensional temperature evolution within a cell due to short-circuit
- Development of an interface module and linking strategy to combine FEA and multi-physical simulation
- Proof of concept by practical application

A combination of structural mechanics and multi-physical simulation will improve result quality significantly and may allow to raise synergies from different simulation models. By this means, every sub-model can work in it's original context without restrictions of any kind.

## 4 Method

The development of the mechanical as well as the multi-physical sub-models has been split up and conducted separately. Basis for both explicit and implicit simulation models are especially designed experiments e.g. dynamic three point bending, nail penetration and high temperature exposure tests. The co-simulation concept has been realised via a tool called *Catalyst* written in Python [27] programming language.

**Mechanical simulation** To reflect the mechanical behaviour of a cell, a simulation model has been set up in explicit FEA code Pam-Crash [28]. This work first has been described by Breiffuss [29] A common cause for short-circuit of electrodes is the puncture of the separator layer. For detailed investigations on the fracture processes of the separator a micro-scale meshing technique has been chosen and is shown in principle in fig. 7. The FEA model has been set up from shell elements modeling the stiffness in normal

direction via contact definitions. Additionally, the friction between the layers has been considered. The structure of the micro-scale mechanical model is shown in fig. 8.

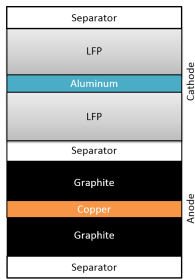


Figure 7: Micro-scale model concept [4].

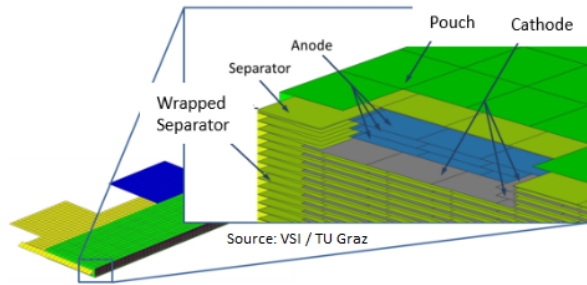


Figure 8: Mesh of the micro-scale cell model [4].

For model validation experiments on component level have been conducted. To determine the active material's share on the overall stiffness bending tests have been performed with the electrode sheets. Tension tests with the pouch foil, the electrodes and the separator have been performed at different feed rates. To get orthotropic material behavior the samples were tested in machine direction (MD), transverse direction (TD) and in 45°-direction (45) as can be seen in fig. 9.[26]

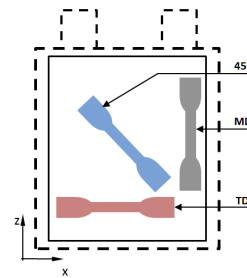


Figure 9: Cell component samples for tension tests [26].

The friction between the cell layers, considering influences of the liquid electrolyte, has been measured using a special built friction test rig shown in fig. 10. These friction tests have been conducted and published by [30]. Additionally, the separator has been subject to puncture penetration test according to ASTM F1306 [31] to improve the separator model quality. The test concept has been outlined by Chen [13] (fig. 11). Corresponding experiments have been conducted and published by Plaimer [15, 16].

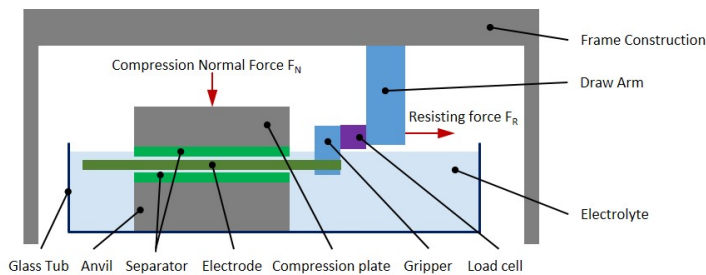


Figure 10: Friction test rig for cell components in wet electrolyte [30].

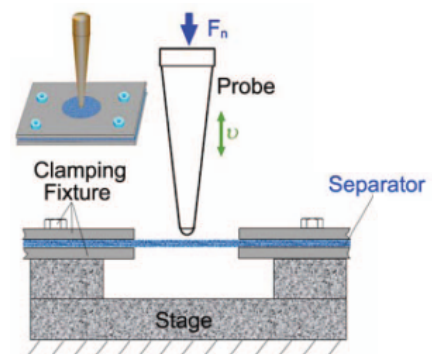


Figure 11: Puncture penetration test of the separator material [13].

**Multiphysical simulation** The multi-physical model is based on an electro-thermal battery simulation approach. This battery model is shipped with AVL FIRE™ [32] and solves the equations for conservation of mass, energy and charge. The active material layers from the mechanical model as well as the

separator layer are combined in AVL FIRE™ to a single "reaction layer" representing the electrochemical processes. Simple models show only one galvanic element surrounded by electrochemically inactive 'thermal mass' as has been used by Feist [26]. In the current work all galvanic elements of the specimen are modeled without the use of thermal replacement mass. To control short-circuit effects a variable ohmic resistance at special interface elements between healthy cell and punctured areas have been set. The major influencing factors of the electrical contact resistance have been identified in experiments (e.g. Volck [33]), modeled mathematically and implemented in AVL FIRE™ as a short-circuit add-on. The actual simulation mesh is shown in fig. 12. The principle of the short-circuit model is depicted in figure 13.

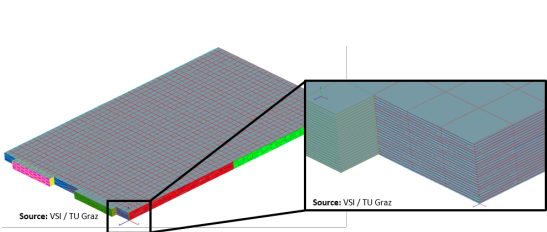


Figure 12: Mesh of the electro-thermal battery model.

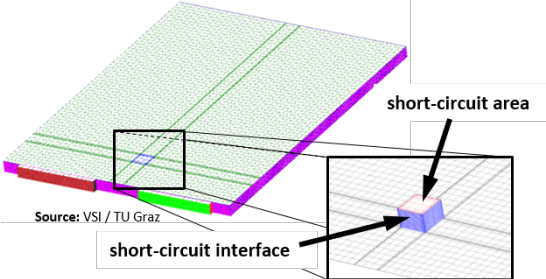


Figure 13: Contact model used to control short-circuit effects at the punctured area.

The parameters for the above described short-circuit model were derived from two series of specially designed experiments. In the first test series ("Smart-Cone") the temperature at the point of short-circuit has been measured. A copper tip with a built-in temperature sensor was driven into the cell (fig. 14). Other than in previous work (e.g. Hatchard [34]) in this paper a cone-shaped penetrator has been used to prevent the separator foil from wrapping around and hence insulating the penetrator tip. A second test series ("Smart-Stamp") showed an enhanced experiment setup using a stamping tool with a defined geometry material sample. A sharp blade stamped out a cube-like piece of the cell and an electrically and thermally insulated material sample including a thermocouple was positioned inside the gap. This allowed to examine the effects of different material properties (e.g. contact resistance) directly at the contact interface. The "Smart-Stamp" principle and a picture of the penetrator is shown in figures 15 and 16.

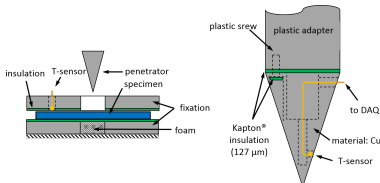


Figure 14: "Smart-Cone" principle.

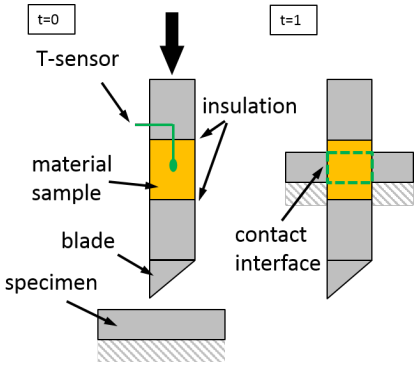


Figure 15: "Smart-Stamp" principle.



Figure 16: "Smart-Stamp" penetrator.

**Geometry interface (co-simulation)** The interface tool *Catalyst* converts the geometry from Pam-Crash into a mesh readable for AVL FIRE™. Because the mechanical model for the separator (isotropic strain rate dependent material) is not suitable for acceptable failure prediction, additionally failure models for the separator can be integrated into *Catalyst* [35]. Failure criteria based on parameters available from the Pam-Crash model (e.g. mechanical strain and stress) are applicable.

The mechanical calculation mesh is loaded into the geometry interface tool and translated to a simulation grid for the implicit electro-thermal solver. Separator elements which have been subject to damage are specially handled and converted to so called short-circuit areas. Afterward, the implicit model solves its equation systems to predict time dependent electro-thermal effects.

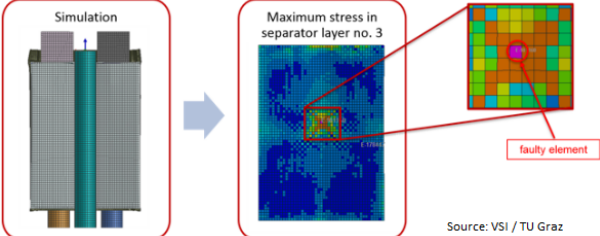


Figure 17: Graphical representation of the mechanical failure criterion.

**Verification Method** To proof the concept a separate series of realistic experiments have been planned and conducted. The test principle is to drive an impactor through the module case, penetrate a cell inside the module and hence cause a short-circuit. For this purpose a generic - close to reality - battery module has been designed. Figures 18 and 19 show the test principle and a CAD rendering of the module prototype.

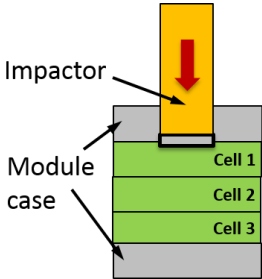


Figure 18: Test principle for the verification experiments.

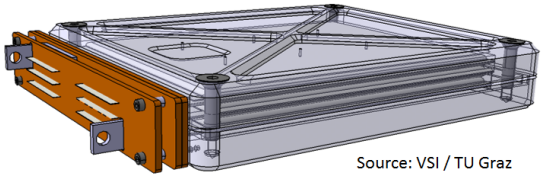


Figure 19: CAD rendering of the generic battery module.

## 5 Results

A FEA model and a multi-physical model have been set up and validated, the geometry interface tool has been programmed and verification tests (battery module tests) have been conducted.

**Mechanical simulation** For the microscopic cell model the dimensions and the material properties of the main cell components have to be known. The main components are current collectors for anode and cathode, active material for anode and cathode, separator and pouch foil. The cell has been disassembled and the geometry of the components has been measured (see fig. 20). The mechanical material properties were determined by tension tests performed at Montanuiversität Leoben [36]. The sample geometry corresponds to fig. 9. The resulting force-displacement graphs can be seen in fig. 21.

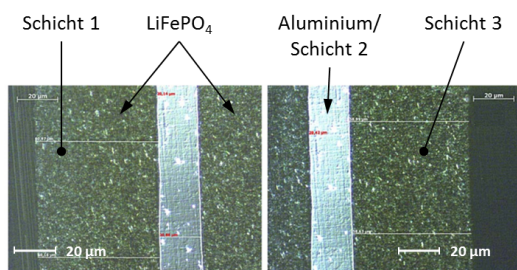


Figure 20: Determination of layer thickness by optical microscopy [26].

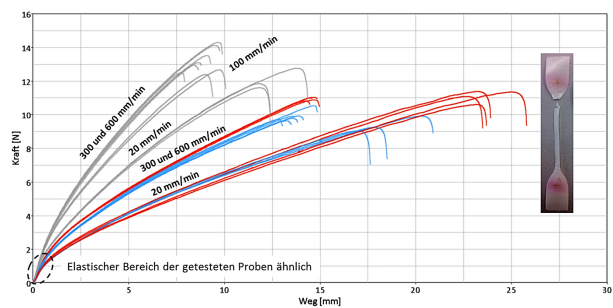


Figure 21: Force-displacement curves for component tension tests. [26].

Using the material properties from the above experiments a micro-scale mechanical simulation model has been validated. For the final verification of the model quasi-static and dynamic tests (3-point bending, indentation and buckling) have been conducted. Figure 22 shows the force-displacement graphs for a 3-point bending cell test whereas the deformation behaviour of the cell model compared to experimental data is outlined in figure 23. A detailed description of this work has been published by Feist [26].

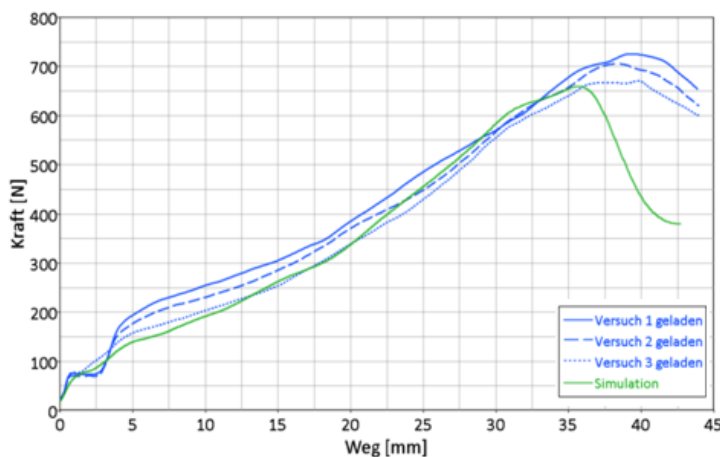


Figure 22: Force-displacement curves for a 3-point bending cell tests. [26].

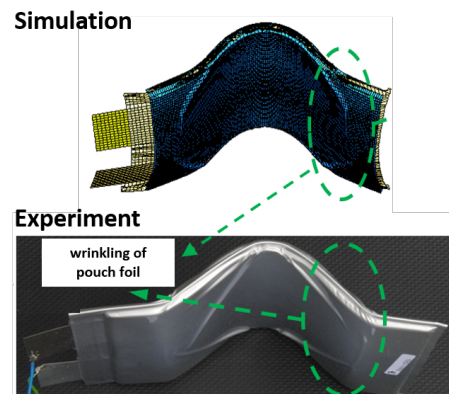


Figure 23: Cell geometry after a 3-point bending simulation and experiment. [26].

**Multiphysical simulation** The multi-physical simulation consists of an electro-thermal battery model (base model) with an add-on short-circuit feature (short-circuit model). To generate realistic output the base model has to be validated for elevated temperature as can occur during short-circuit events. A test matrix (fig. 24) for cell discharge experiments has been processed resulting in cell voltage curves for relevant ranges of discharge current and ambient temperature. Using these curves parameter generation for the base model has been done via an in-house software tool from AVL. The results of discharge experiments in comparison to discharge simulation are depicted in figure 26. Another important finding from these tests is the maximum ambient temperature the cell can withstand without obvious mechanical damage. While cell swelling occurs at about 110 °C (orange in fig. 24), venting occurs at about 120 °C (red in fig. 24). A specimen after venting is shown in fig. 25.

Temperatur [°C]	C-Rate [-] bzw. Strom [A]					
	0,5	1,0	2,0	3,0	4,0	5,0
25	10	20	40	60	80	100
40						
60						
80						
100						
110						
120						

Figure 24: Test matrix for high temperature cell exposure tests.



Figure 25: Specimen after high temperature exposure (> 100 °C).

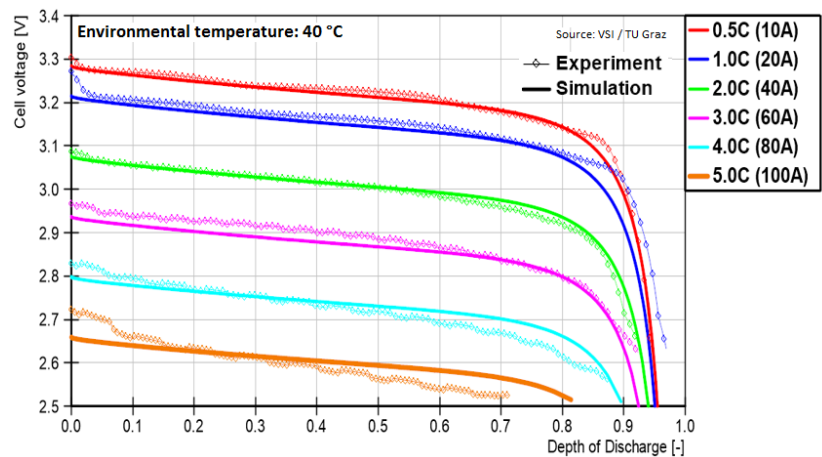


Figure 26: Discharge curves from experiment and simulation at 40 °C.

To find out what happens at the short-circuit spot a series of special experiments has been conducted. The penetrator punctured the cell and the temperature in the spot has been measured. A test matrix has been processed including variation of feed rate and penetrator displacement. The experiment setup for "Smart-Cone" and the temperature evolution at the copper tip are depicted in figures 27 and 28.



Figure 27: Test situation for "Smart-Cone" cell penetration tests.

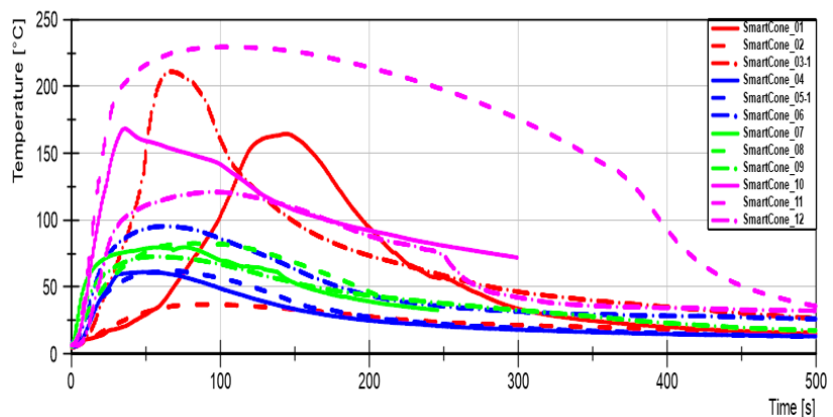


Figure 28: Temperature evolution of the copper tip during "Smart-Cone" tests.

For the "Smart-Stamp" test series the sample geometry (sample length: 10, 15 and 20 mm) and sample

material (steel, phenolic paper, polyoxymethylene (POM-C)) has been varied and the sample temperature has been measured. The temperature evolution in the spot of short-circuit can be seen in 29. Fig. 27 shows a picture of a tested specimen.

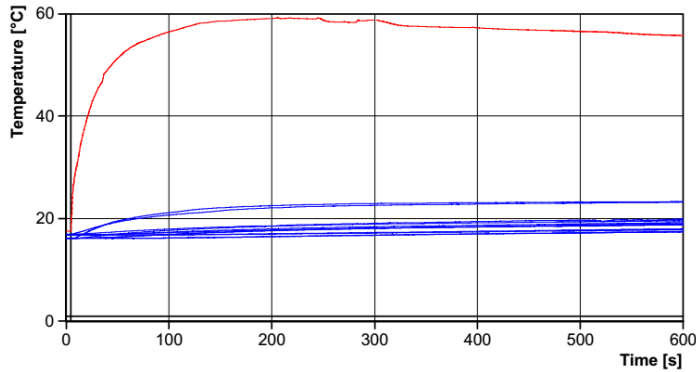


Figure 29: Temperature evolution of the material sample (red) and the cell surface (blue) during "Smart-Stamp" tests.

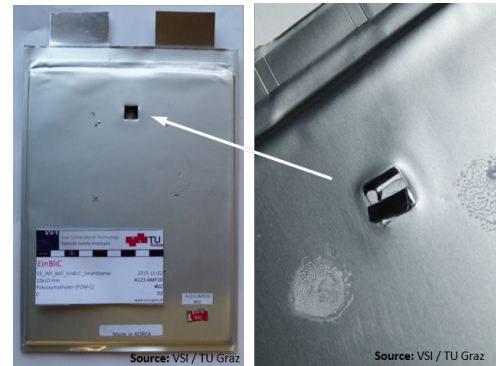


Figure 30: Specimen after "Smart-Stamp" test.

Knowing the geometry and the material properties of the sample and the heat rate from the measurement an ohmic resistance can be derived. This generic short-circuit resistance is supposed to cause the heating of the sample and hence represents a main parameter for the short-circuit model. For all conducted experiments the temperature evolution has been related to the particular surface area in contact (short-circuit interface). Further considering the material parameters of the sample (e.g. specific ohmic resistance) this gives a normalised, material independent heating-power-per-area value. In figure 31 a measured temperature rise during a "Smart-Stamp" experiment is depicted, whilst figure 32 shows a typical surface-specific heat release curve.

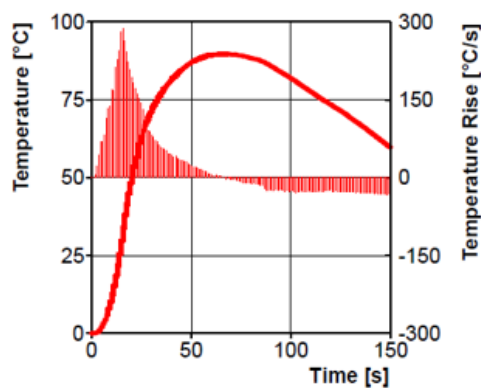


Figure 31: Example for a heat release curve in the spot of short-circuit.

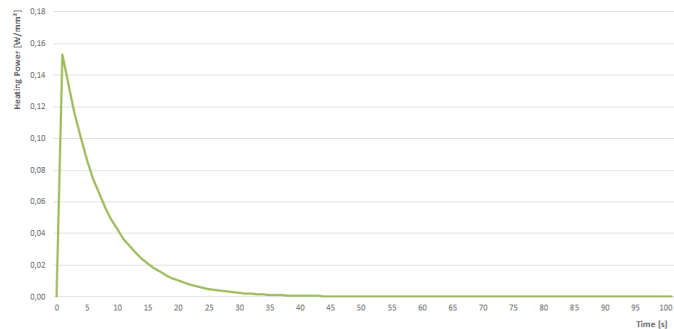


Figure 32: Typical shape of a heat release curve at the short-circuit interface.

$$P(t) = \Delta P \cdot t \quad | \quad P < P_{max} \quad (1)$$

$$P(t) = P_{max} \cdot e^{-\frac{t}{\tau}} \quad | \quad P \geq P_{max} \quad (2)$$

Equations 1 and 2 show the mathematical description of the normalised heat release curve. This short-circuit model has been implemented in Fortran programming language and embedded in AVL FIRE™ via "user functions". At every simulation time-step for every mesh element in the short-circuit interface a certain heating power according to the short-circuit model is prescribed. This is done by setting a corresponding electrical resistance for the interface element. The resistance causes an electric current from

the cell through the interface into the short-circuit area and hence induces an ohmic heating in the spot. This represents the local heating due to short-circuit.

**Proof-of-concept tests** To verify the submodels as well as the whole simulation work-flow a series of tests have been accomplished. A steel impactor was driven through the casing into the generic module prototype and penetrated the topmost of three serially connected cells inside. This caused an exothermic reaction as can be seen in Fig. 33.



Figure 33: Exothermic reaction during module test no. 2

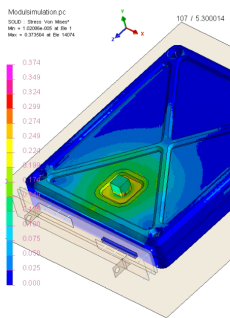


Figure 34: Mechanical stress on the case in module test simulation.

The same test configuration has been set up as a mechanical model in Pam-Crash. Then *Catalyst* applied a separator failure criteria translated the mesh. The basis for failure detection has been the simulated mechanical stress (see fig. 34). Subsequently structural and geometrical information from Pam-Crash has been passed on to AVL FIRE™. The so generated cell geometry including a short-circuit area has been used to simulate the electrical-thermal response of the cell. The measured temperature rise in the spot of short-circuit during all three tests (grey shaded corridor) is shown in comparison to the simulated temperature evolution (blue line) in Fig. 35. The voltage drop during the experiments (grey shaded corridor) compared to the simulation of the electrical response of the cell in the simulation (blue line) is depicted in fig. 36.

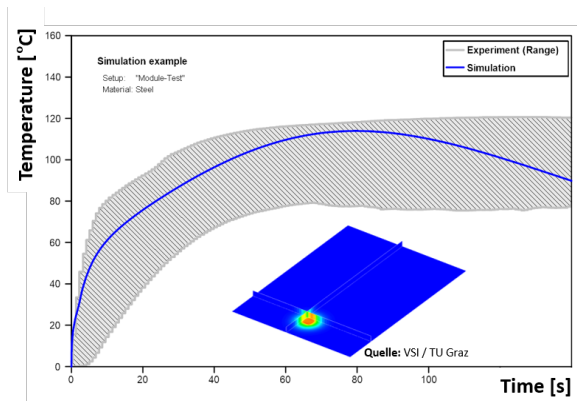


Figure 35: Experimental data (grey) in comparison to simulation results (blue)

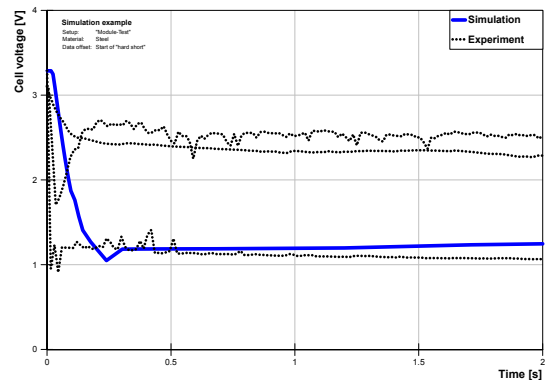


Figure 36: Experimental data (grey) in comparison to simulation results (blue)

## 6 Conclusion

By now few has been published about combined explicit and implicit battery simulation models. This paper presents the development processes for a simulation work-flow based on a concept first published by Feist [26] in 2013. The concept has been enhanced and the sub-models have been developed further. An explicit finite element code depicts the mechanical stress in the cell's calculation elements. In a geometry interface this information is examined by a mechanical failure algorithm and passed on to a multi-physical simulation where possible electrical and thermal effects are computed. This semi-automatic co-simulation work-flow (fig. 37) is able to predict the time-dependent mechanical, electrical and thermal behaviour of Li-ion batteries due to crash loads in detail. A series of mechanical abuse tests with a generic battery module has been conducted. The test scenario has been reproduced in the simulation to proof the concept. Simulation results showed excellent conformity with the experimental data.

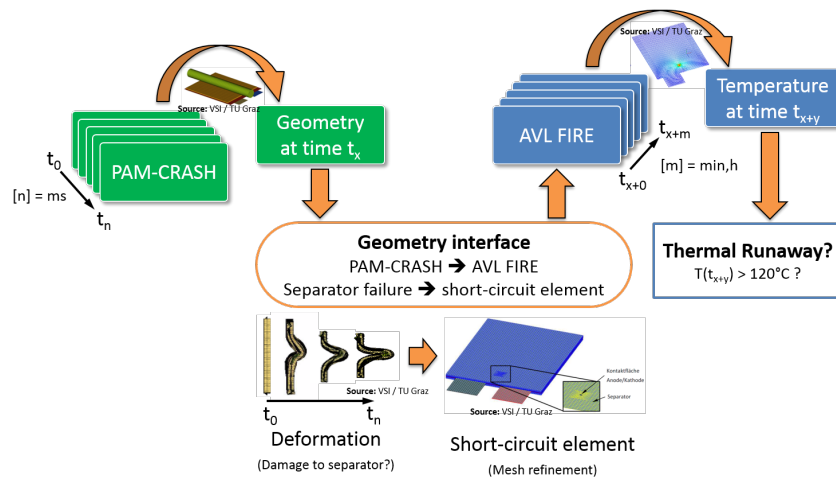


Figure 37: Co-simulation of explicit FEA (Pam-Crash) and implicit multi-physical (AVL FIRE<sup>TM</sup>) solvers.

The following list states a potential scope of application for the presented simulation solution:

- Estimation of the thermal runaway risk for a given mechanical load scenario
- Prediction of the maximum allowable deformation for a cell without risking thermal runaway
- Safety assessment of design variants and installation layouts of battery cells, modules and packs
- Assessment of thermal runaway avoidance and mitigation measures (e.g. cooling system)
- Derivation of product specs for cell manufacturers to enhance the cell's intrinsic safety

Future developments should try to improve prediction quality. The present model can give a statement whether a thermal runaway may start or not. A precise prediction of the hazard level [37] is not applicable at the moment. Therefore the electro-thermal simulation would have to be extended by e.g. reaction kinetics and/or gas diffusion models.

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## Author

### **Dipl.-Ing. Simon Franz HEINDL**

*Vehicle Safety Institute, Graz University of Technology, Inffeldgasse 23/1, 8010 Graz, Austria*

*[simon.heindl@tugraz.at](mailto:simon.heindl@tugraz.at)*



Simon Franz Heindl joined Vehicle Safety Institute as University Project Assistant in 2013. Area of work are safety aspects of traction batteries for electric vehicles. Main focus is on numerical simulations of multi-physical (electrical, mechanical, thermal) effects of Li-ion cells during short-circuit events.