Novel Method for the Three-Dimensional Simulation of Mechanical Ageing of Battery Modules

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Abstract: This study introduces a novel method for modelling the mechanical ageing behavior of battery modules over lifetime, based on a simplified, mathematical approach. The focus is placed on the force displacement behavior of battery modules due to the swelling of its cells in the course of electrochemical ageing. In the first step, the development of a proper modelling method is conducted, before the implementation of the single-domain model is carried out. Multiple size scales are included in this model, since cell and battery module level are considered. The model implementation is realized with two different approaches for examination of simulation trade-offs regarding accuracy and computing time. In the first approach, the module is modelled using the Finite-Element-Analysis (FEA) with a high number of elements. In an alternative, more simplified approach, the module model in form of a mathematical, analogous model is implemented with a significantly fewer number of elements. In both cases, the model layout is similar. Finally, both the approaches are validated with experimental measurements and compared regarding accuracy and computing time, amongst other parameter.

1 INTRODUCTION

The Volkswagen Group is committed to the Paris Agreement and is determined to be climate-neutral until 2050 (Mortsiefer et al., 2019). The agreement was signed in 2015 by the world community and supports the containment of anthropogenic greenhouse gas emissions and fight climate change (Bundesministerium für Umwelt, Naturschutz und nukleare Sicherheit, 2017). A high market share of battery-powered electric vehicles (BEV) has the potential to make a significant contribution to this agreement. A changed and more environmentally conscious customer behavior has even more lifted this issue and can be observed by the steadily rising number of new vehicle registrations of BEVs (Kraftfahrt-Bundesamt, 2020).

The motives for acquiring a battery-powered electric vehicle are diverse. In contrast to conventional vehicles with an internal combustion engine (ICEV), the benefits of BEVs for their immediate environment are enormous. In addition to being able to drive locally emission-free (Holstenkamp & Radtke, 2018) and having an at least twice as high well-to-wheel efficiency, there are numerous more benefits to add (Doppelbauer, 2020).

Then again, BEVs must increase their optimization potentials to be able to compete with conventional vehicles. Even though BEVs shorten the gap, ICEVs still lead in multiple disciplines like driving distance and acquisition costs (Frenz, 2019).

Special attention must be paid to the high-voltage battery system of a BEV, since it is the costliest component of its power train (Frenz, 2019; Sterner & Stadler, 2017). A common assembly of a battery system is portrayed by the modular composition of it. Here, lithium-ion battery cells are electrically connected and integrated into a housing to form a battery module (Dörnhöfer, 2019; Korthauer, 2013). The integration of the battery module into a battery system takes place in the next step (Dörnhöfer, 2019; Korthauer, 2013). Due to the electrochemical degradation of the built-in battery cells over lifetime, they experience changes not only on their electrochemical but also on their mechanical level (Broussely et al., 2005; Cannarella & Arnold, 2014;

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Kampker et al., 2018; Korthauer, 2013; Sterner & Stadler, 2017). In addition to a continuously decreasing capacity and an increasing internal resistance, the ageing of the cells is also expressed through thickness increase, involving a corresponding swelling force over lifetime (Bitzer & Gruhle, 2014; Cannarella & Arnold, 2014; Grimsmann et al., 2017; Korthauer, 2013; Li et al., 2020; Sterner & Stadler, 2017). As a result, the swelling of the battery cells is transmitted on to module level. It has been shown by using experiments and simulations with a simplified module setup that the module swells while overcharging its cells (Jeon et al., 2007). In the process, it was possible to measure the deformations of the module endplate over time (Jeon et al., 2007). Therefore, it can be reasoned that the swelling of the cells due to their electrochemical degradation will also lead to significant deformations on module level. It has also been depicted by elaborate and time-consuming FEA-simulations that this behavior over lifetime can be expected (Choi et al., 2018). When integrating the module into a battery system, e.g. by fixing it with screws, its ageing behavior with changing dimensions over lifetime sets a relevant challenge. In order to effectively and safely design a battery system with a modular composition, the swelling behavior of its modules has to be known in advance.

Consequently, an analysis on the mechanical ageing behavior of battery modules is necessary for prevention of integration problems. Due to the time-consuming and costly testing of battery module swelling behavior, the benefits of a simulation model are obvious. In this study, a novel method for simulating the spatially resolved mechanical ageing behavior of battery modules of multiple size scales over lifetime is introduced, which is based on a simplified, mathematical approach. It is for the first time that a mechanical ageing model for modules is also validated against experimental data, according to the best knowledge of the authors. The model is built for a module consisting of lithium-ion pouch cells.

2 METHOD DESCRIPTION

Since this study solely focuses on the mechanical behavior of battery modules, single domain modelling is applied. In addition, a multi-scale approach is chosen for the model, because it is also supposed to make spatially resolved predictions about swelling and displacement at cell and module level. While the smallest scale in the model is at component level, represented by cells and pads for example, the largest scale is the battery module.

The key aspect of the model is a deformation analysis of the module and all its components over lifetime, caused by swelling of the built-in cells due to their electrochemical degradation. The developed method for simulation of the mechanical ageing behavior of battery modules contains multiple steps, which need to be conducted in the order specified (Figure 1). In the first step, a three-dimensional (3D) model of the examined battery module is built in a corresponding simulation program and discretized into finite elements. The model includes all connections and components of the module, like cells and cushion pads, and arranges them like in the real module assembly. Afterwards, components and connections are calibrated and parameterized according to their real material behavior. This includes the specification of material properties like young’s modulus or even force-displacement curves of applied components. In the third step, a cell swelling model as a function of cycle dependent volume increase per discretized finite element is built, based on experimental lifetime measurements. The swelling model of the cell is then implemented for each cell in the module model. After the set-up of the model is completed, the simulation of the mechanical ageing behavior of the module is executed in the last step. In this process, swelling, displacement and mechanical stress of the cells and other components is spatially resolved simulated, resulting in a deformation and displacement of the module endplates.

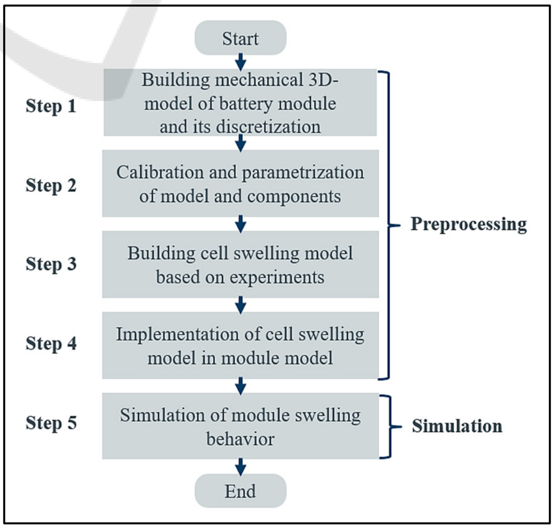

Figure 1: Schematic representation of the simulation method for swelling prediction of battery modules.

3 MODEL DEVELOPMENT

A main issue that must be considered in the development of simulation models is the conflict of their accuracy and computing time. Complex models with a high number of elements promise accurate results, however they also bring a high computing time with them. Simplified simulation models with a significantly fewer number of elements, on the other hand, execute quickly, but may lack in accuracy. Another aspect that is equally important as accuracy and computing time of the simulation model is the time spent for building a model configuration as well as its design flexibility. The examination of this issue represents a further priority of this study next to the previously described method.

In the light of the above mentioned aspects, the development of the model according to the described method is realized with two different approaches. The first approach focuses on a complex simulation of the battery module with a high resolution and number of elements. For this case, a commercial FEA software is used. In an alternative, more simplified approach, the method is realized by a mathematical, analogous model, which is based on a reduced set of mechanical equations. This approach has a significantly reduced number of elements and equations in comparison to the complex FEA. In the following two subsections, the model development with each approach is separately depicted.

3.1 Finite-Element-Analysis

The commercial software Abaqus FEA is used for the model building and subsequent simulation of the battery module. The finite-element-method is well suitable for multi-body-simulation and therefore it fits for the simulation of a battery module, which consists of numerous components like cells, pads, endplates and other. As described, the aim of the simulation with this approach is to have a high resolution of the spatially resolved swelling behavior of the module over its lifetime. For that reason, each component of the investigated battery module is modelled in 3D and parameterized at first. Modelled components of the battery module are its cells, cushion pads, module frame, endplates, thermal resin and busbars, amongst other things. In the next step, the components are assembled the same as in the examined module (Figure 2).

FEM-simulation is based on the setup and solution of a system of equations, which are based on physical laws ("Dubbel Taschenbuch für den Maschinenbau 1: Grundlagen und Tabellen", 2020). The size of the equation system and therefore the computing time mainly depend on the number of finite elements configured in the meshing process ahead of the simulation. Therefore, the resolution of the battery module by finite elements is accordingly chosen to find a good compromise between computing time and accuracy (Figure 3).

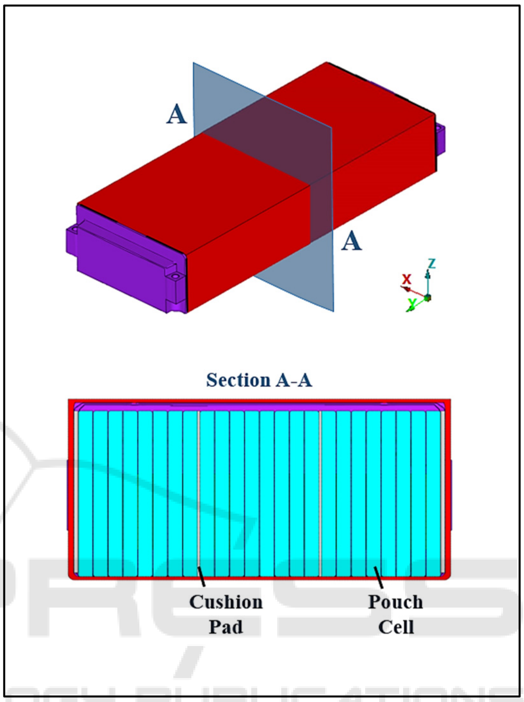

Figure 2: CAD-model of the examined battery module.

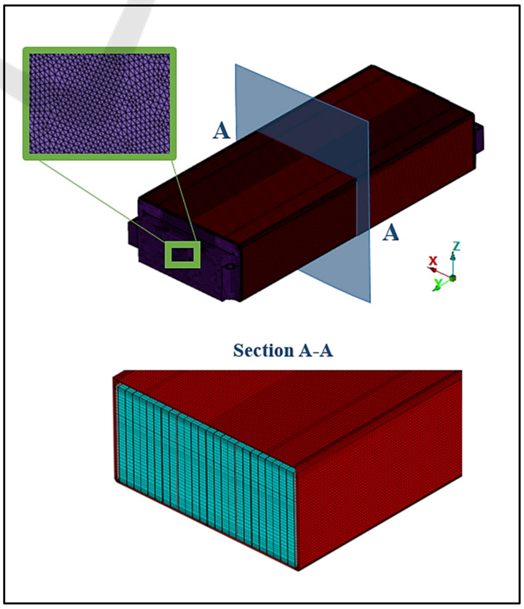

Figure 3: Meshed model of the examined battery module.

In order to implement the swelling behavior of the built-in cells in step 3, it has to be experimentally determined at first. For that reason, the examined cell is placed in a test jig and cycled several hundred times, building up a steadily growing swelling force. In this process, the swelling force of the cell is measured, using a load cell.

The measured cell swelling data is used for building a swelling model for the cell, which is then implemented into the FEM-model in the last step of the pre-processing process.

3.2 Simplified, Mathematical Modelling

A mathematical, analogous model for the mechanical ageing behavior of battery modules has been developed in the commercial software MATLAB as an alternative approach to the complex FEM-software. The focus of this approach is to accelerate the model building process as well as to reduce the computing time, while maintaining model accuracy.

The model is based on an algorithm, which is capable of automatically discretizing a module into finite elements and building up a corresponding mathematical equation system, describing the three-dimensional mechanical interaction behavior of the elements by physical laws. The equation system can be described in matrix notation as following:

$$\{F\} = [K] \cdot \{u\} \tag{1}$$

Here [K] stands for the global stiffness matrix, whereas {F} for the global force and {u} for the global displacement vector:

$$\begin{Bmatrix} F_1 \\ \vdots \\ F_n \end{Bmatrix} = \begin{bmatrix} K_{11} & \cdots & K_{1n} \\ \vdots & \ddots & \vdots \\ K_{n1} & \cdots & K_{nn} \end{bmatrix} \cdot \begin{Bmatrix} u_1 \\ \vdots \\ u_n \end{Bmatrix} \tag{2}$$

In this way, it resembles the computing process of FEM-software, but it distinguishes itself by using a reduced and simplified equation set. In the mathematical modelling, the algorithm needs information about the module, its assembly and material properties of the components as well as general model information like the chosen number of finite elements and the discretization of the module model. The input data are entered via a user interface according to the data of the investigated battery module. In comparison to the FEM-approach, a fewer number of elements is chosen in this process to create the battery module model; hence, it is very efficient in terms of computing time. Further information regarding module and component geometry and assembly and their material properties must also be provided in the user interface. Due to the wide number of selection options in the preprocessing process, the developed model offers maximum flexibility for modelling battery modules of different geometries, assemblies, materials, cells and further characteristics. A geometric visualization of the configured battery module is also available for verification of the input data. Furthermore, the model can accommodate the experimentally determined swelling behavior of individual battery cell as the input boundary conditions, representing step 3 of the pictured method in Figure 1. After setting up the model parameters and input data, all the components of the battery module are created as 3D link elements with linear interpolation and thus the complex model can be simplified by using a mathematical system of equations. The simulation model then solves the system of mathematical equations to illustrate the swelling behavior of an entire battery module as well as its components over lifetime. Finally, the visualization of the deformed module geometry with the representation of displacement, tensions and compressional forces using different colours are implemented for the meaningful interpretation of simulation results.

3.2.1 Interim Analysis Regarding Preprocessing

The preprocessing of the two approaches differs significantly. The simplified, mathematical modelling technique allows the user an easy use regarding model building due to the practical user interface. As described in section 3.2, it also spares the user the long-lasting component modelling, parametrization and subsequent module assembly and meshing process (Figure 4). Instead, the user simply needs to provide the required input information by filling out an interface and the algorithm takes care of the rest. This way the simplified model is even predestined for the use in optimization studies as well.

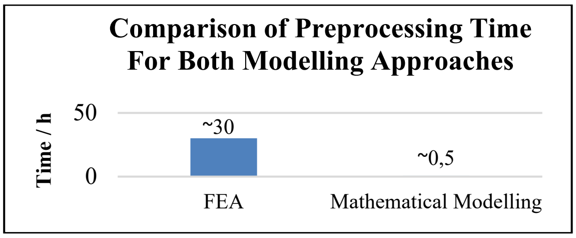

Figure 4: Comparison of preprocessing time for both modelling approaches.

4 EXPERIMENT

A pouch module, consisting of 24 electrically connected cells, is used for the experimental investigation. The experimental setup for the mechanical ageing test and its functionality is schematically illustrated in Figure 5. The investigated battery module is placed in a temperature chamber and fixed on a metal surface. Afterwards, it is equipped with distance sensors on specific locations on its surface (Figure 6). The module inside the chamber is conditioned to an elevated room temperature for accelerated ageing and swelling behavior and then cycled by the battery cycler with a constant current rate for several hundred cycles. During the entire time, the deformation of the module is measured by the applied distance sensors.

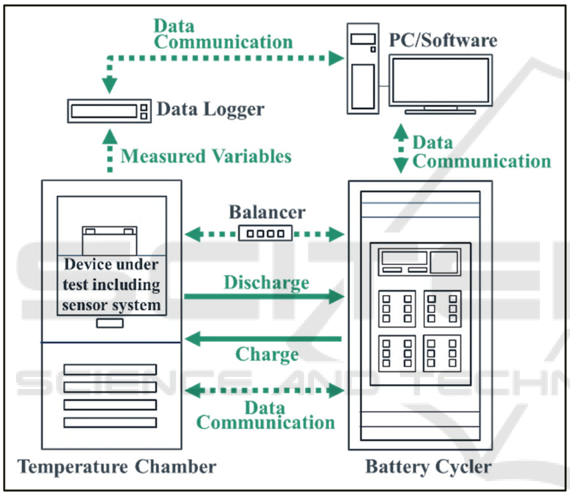

Figure 5: Experimental setup for deformation measurement of battery modules.

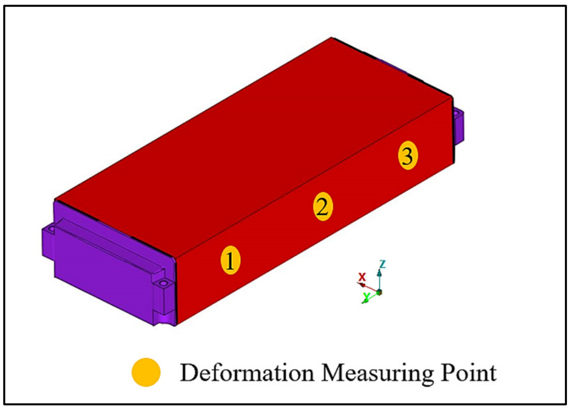

Figure 6: Swelling measurement points on device under test.

5 RESULTS

The results of the experiment are shown in Figure 7. The graphic shows a comparison of the deformation at the measured positions. It is noticeable that Position 2 clearly experiences more deformation in comparison to Position 1 and 3 and therefore a bulging of the module frame takes place. Furthermore, the experimental data reveal that the module has a high slope regarding swelling during the first 100 cycles, before the slope decreases and becomes linear for the following several hundred cycles. Position 2 experiences a larger deformation due to the fact, that the module frame has a lower stiffness in its center section in comparison to the sections closer to side, where it is welded to the endplates, which increase stiffness and stability.

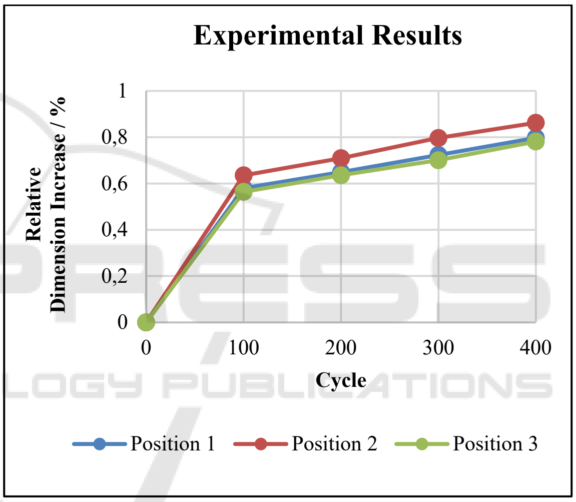

Figure 7: Experimental results for battery module swelling.

The module swelling simulation by both FEA and simplified, mathematical approach deliver good results over lifetime, which are close to the experimental data. A comparison of the relative dimension increase at Position 2 is shown in Figure 8. The deviation between FEA and experiment is under 10% over the entire 400 cycles. A major benefit of the FEA is its ability to simulate non-linear material behavior. On the other hand, the simplified, mathematical approach is currently limited regarding this aspect and only allows cycle-independent, constant material behavior, which is depicted by the green line in Figure 8. A further simulation is conducted with the simplified model by adapting its cell material behavior, in order to compare its ability regarding accuracy to the FEA. In this case, the cell stiffness in the simplified approach is firstly parametrized with the same value, which was used in the FEA for 100 cycles. In the next step, the increase of cell stiffness for the next 300 cycles is determined in the FEA and then applied by a corresponding function in the simplified model. By doing so, the dark blue line in Figure 8 clearly brings out that the simplified approach also can accurately predict module deformation even in the later stages of cycling and that cell material stiffness has a great influence on the prediction of the module deformation. Remaining differences after 100 cycles presumably arise from non-linearity of further module components.

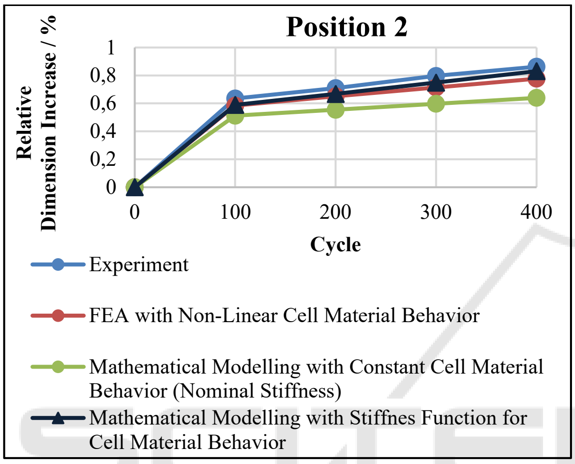

Figure 8: Comparison of battery module relative dimension increase in experiment and simulation at position 2.

In the following Figures 9 and 10, a comparison between battery module normalized dimension increase in experiment and simulation is shown.

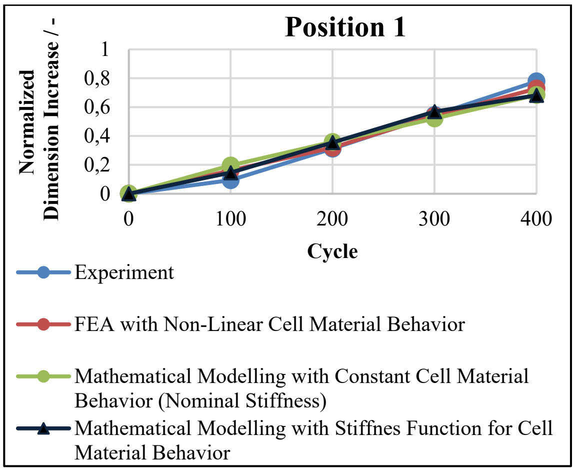

Figure 9: Comparison of battery module normalized dimension increase in experiment and simulation at position 1.

Figures 9 and 10 confirm that the results of both simulation approaches correspond well with the experiments on all positions over lifetime. They also confirm the linear characteristic of the current simplified, mathematical approach and simultaneously reveal its optimization potentials due to its limitations regarding that.

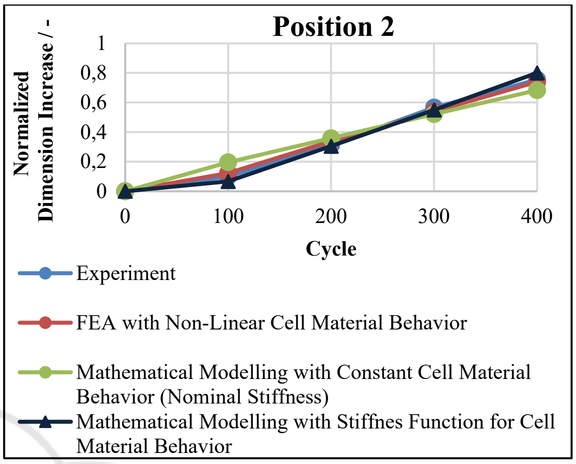

Figure 10: Comparison of battery module normalized dimension increase in experiment and simulation at position 2.

Regarding computing time on the other hand, the simplified mathematical approach shows his real potential due to the small number of finite elements used for the simulation (Figure 11).

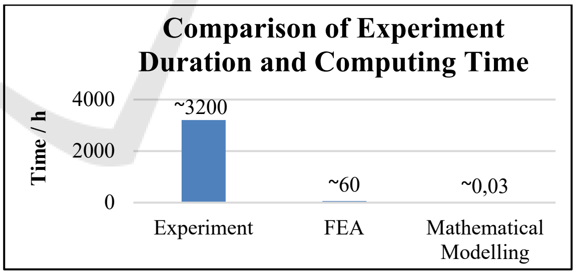

Figure 11: Comparison of computing time and experiment duration.

6 CONCLUSION

A novel method for predicting the spatially resolved mechanical ageing behavior of battery modules over lifetime has been developed and implemented, which is based on a simplified, mathematical approach. Additionally, the method has also been realized with a complex FEA for comparison purposes, especially regarding accuracy and computing time. For assessment and validation of the developed models, an experimental study was conducted, where a high voltage battery module consisting of 24 electrically connected lithium-ion pouch cells was exposed to elevated temperatures for accelerated electrochemical degradation and swelling of its cells and cycled several hundred times. During the cycling, it was equipped with distance sensors, which measured the spatially resolved deformations of the module from the outside. The recorded data of the module swelling due to electrochemical ageing was then compared to the simulation results. According to the best knowledge of the authors, this has been the first time a mechanical ageing model for modules has been validated against experimental data. The first set of simulation results of both modelling techniques has proven their ability to predict the spatially resolved module swelling behavior over lifetime with good accuracy. The simplified model in his current working status works well for fast predictions. It is also suitable for optimization studies due to the developed algorithm, which automatically builds up mechanical models for different module designs and configurations by using data, which are entered in a user interface. On the other hand, the FEA delivers accurate results with a higher resolution, but with a longer preprocessing and computing time. In comparison to the real experiment, which took about four and a half months, both model approaches can reduce this duration massively.

7 OUTLOOK

The optimization of the simplified, mathematical approach is ongoing, in order to extend its simulation abilities, like the simulation of non-linear material behavior, in order to reach higher accuracy. In the process of that, the model equations are being optimized by taking into account further in-depth physical effects. In addition, sensitivity studies regarding the number of finite elements are being conducted.

Further experimental and simulative studies for different module types are also ongoing. In doing so, the modelling of prismatic battery modules is also being realized.

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