Two Modelling Approaches of Lithium-Ion Pouch Cells for Simulating the Mechanical Behaviour Fast and Detailed

Alexander Schmid[1], Marco Raffler[1], Clemens Dünser[1], Florian Feist[1], Christian Ellersdorfer[1]

[1]Vehicle Safety Institute, Graz University of Technology

Abstract

For the simulation of the mechanical behaviour of pouch cells, there are varieties of modelling approaches, which differ greatly in the level of detail. In macroscopic models the single plies constituting the cell are not discretized separately, but are homogenized in thickness (pouch cell) or in radial direction (cylindrical cell), respectively. The main advantage of macroscopic models lies in their computational efficiency. However, these models fail in predicting short-circuit on a component-based level. Determination of the component behaviour is only possible to a very limited extent, which means that a component-based short-circuit criterion is also not an option.

Modelling approaches that depict each single ply provide more thorough insights in the loading, damage and failure of single cell components, that might ultimately lead to internal short circuit and cell failure. This higher level of detail comes with higher computational effort due to high number of interlaminar contact interactions and small characteristic element length.

Both types of modelling have their justification and are used in different situations.

Two approaches are presented here. The first, the ‘Simplified Applicable Model’ – SAM, is a macroscopic approach. It aims at ensuring not only computational efficiency but also adaptability. This model is to be used primarily in the field of full-vehicle simulation. The mechanical response to loads needs to be calibrated against cell experiments.

The second approach, the ‘Detailed Layer Model’ – DLM, is a layer-by-layer approach, where the structural cell response arises from accurate modelling of each single layer. This model is particularly suitable for in-depth investigations on cell component level. Despite the high level of detail, the computational effort was kept as low as possible, e.g. by dispensing interlaminar penalty contacts.

The different concepts, characterisation tests and short-circuit criteria are shown alongside the simulation results.

1 Introduction

A pouch cell consists of multiple stacks of “plies” which are denoted as anode, separator and cathode. The stacks are immersed in an electrolyte and surrounded by a flexible “coffee-bag”-like casing denoted as pouch. The electrodes, i.e. anode and cathode themselves can be considered a laminate of metallic current collectors (aluminium or copper) and active material coating (mainly carbon). The pouch is a laminate, too, consisting of an aluminium foil covered with a polymer.

A contemporary pouch cell can consist of around one hundred layers, with a thickness of 20-100µm, each. Obvious, that these plies are vulnerable to mechanical loading.

Mechanical loading of lithium-ion pouch cells can have far-reaching consequences. Overloading can damage the separators (layers between anodes and cathodes), which can lead to an internal short circuit and thus to a so-called thermal runaway. These cells react very sensitively, especially to transverse pressure, i.e. loads normal to the electrode plane. The deformations in transverse compression that can be tolerated are far lower than in bending or in-plane loads.

There are different approaches to model the mechanical behaviour of such energy storage systems. Macroscopic approaches consider the cell as a homogeneous body ([1] , [2]) and often neglect cell features like anisotropy and strain rate dependency. These are distinguished above all by high computational efficiency. In contrast, detailed approaches take into account the individual components of a cell ([3] , [4]). Accordingly, the computational effort is many times higher. However, they also have a higher degree of detail.

The main problem in heterogeneous modelling of pouch cells results from the large number of thin layers that have to be modelled. Since the Courant criterion must be fulfilled for stable calculations in explicit FEM, the layer thickness has an influence on the time step. The separator is the thinnest layer with only about 20µm. Besides the layer thickness, the contact modelling is also a major hurdle. In this paper, a 41Ah NMC cell is investigated. The jelly stack consists of 85 layers of anodes, cathodes and separators. [5]

Two models of the lithium-ion pouch cell are presented. In both, the macroscopic variant and the layer-by-layer approach, special focus is given to the behaviour in the thickness direction. Both models were created with the commercial software LS-DYNA.

2 Detailed Layer Model – DLM

Our model with the heterogeneous approach is called Detailed Layer Model and aims at a profound analysis of the cell behaviour under mechanical load. The main advantage here, apart from the level of detail, is the transferability: Large parts of the overall structural behaviour arises from the behaviour of the individual components. This reduces the effort for characterisation experiments on cell level and allows for parametric studies, such analysis of cell-shapes, ply thickness, cell dimension and material properties.

2.1 Concept

The basic concept of the Detailed Layer Model is shown in Fig. 1; shells and solid elements represent the jelly stack. The shells represent the in-plane behaviour of the individual components. Alternating with these are solids, replicating the out-of-plane behaviour. This includes the transverse pressure, the shear behaviour and the interlaminar interaction. The individual layers are connected by ***NODE_MERGE_SET**. If two nodes are within the defined tolerance, they are replaced by a new single node.

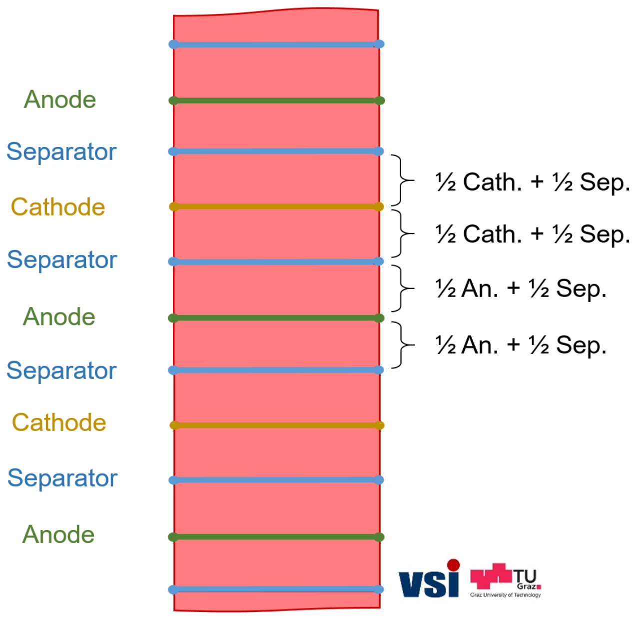

Fig.1: Concept of the Detailed Layer Model

The modelling deliberately dispenses interlaminar penalty contacts, to increase the computational efficiency and the robustness.

2.2 In-Plane Behaviour

The in-plane behaviour is represented by the shell elements. Tensile tests of the individual materials are required for characterisation. For this purpose, samples are extracted in different directions. The samples for anode and cathode are extracted in machine and cross direction. For the separator and the pouch foil, the intermediate 45° direction is tested, too. The samples are tested at two loading velocities (20mm/min and 600mm/min), to identify influence of the strain rate in addition to the anisotropy. The tests were carried out five times each for statistical validation. For anode and cathode, both, the results showed neither anisotropy nor a recognisable influence of the strain rate. With the pouch foil, the influence of loading direction was found negligible. Therefore, all three materials, i.e. electrodes and the pouch, are assumed isotropic and were modelled with ***MAT_PIECEWISE_LINEAR_PLASTICITY**. The modelling of the failure is done by ***MAT_ADD_EROSION**. The required values of the failure strain also come from the tensile tests. In contrast, the behaviour of the separator is more complex. The test results show a significant anisotropy as well as a strain rate influence. The failure strain is also dependent on orientation and loading rate. Physically, this behaviour could be explained by the manufacturing process [6], where the pores for ion-conduction, is created through pre-stretching. The material model

***MAT_EXTENDED_3-PARAMETER_BARLAT** is used here. This makes it possible to define the material behaviour in machine, transversal and diagonal directions at different strain rates. In combination with the damage model ***MAT_ADD_GENERALIZED_DAMAGE**, all determined properties can be reproduced.

2.3 Out-of-Plane Behaviour

The out-of-plane behaviour is represented by the solid elements. This includes the behaviour in thickness direction as well as the shear of the components and the interlaminar contact. Since the shells already cover the in-plane behaviour, the solids must not show any influence here. This means that a decoupled material model is required. For this purpose, ***MAT_MODIFIED_HONEYCOMB** is used. This additionally offers the possibility of a discrete element formulation with ***SECTION_SOLID** ELFORM 9. In that way a constant time step, even under severe compression, can be achieved. Especially for simulations of transverse pressure, this has a positive effect, as the already thin elements are further compressed. In contrast to the shell elements, they are not characterised by component tests but derived from cell tests. The test configurations, which are used, are shown in Fig. 2 with the results.
Fig. 2a shows the cylindrical indentation test, which can be used to determine the transverse pressure behaviour. This behaviour is distributed equally among all solid elements. (Remark: In another variant, which is not discussed here, the transverse compression behaviour was assumed heterogeneous, i.e. separator and electrodes differed w.r.t. their mechanical behaviour in transverse compression.) The cumulative shear properties (component and interlaminar contact) are determined iteratively by simulating a 3-point bending test, which is shown in Fig. 2b.
The influence of the electrolyte was taken into account in this model through ***AIRBAG_LINEAR_FLUID**. The enclosed volume of the pouch was selected and assumed incompressible.

2.4 Results

Fig. 2 shows the results of the characterisation tests in numerical and physical environment side-by-side. In the cylindrical indentation test, an impactor with a diameter of 30mm loads the cell longitudinally. In the real test, the drop in cell voltage is indicative of the internal short circuit. The experimental and numerical force-displacement curves correlate very well. The simulated failure of the separator also matches with this value from the quasi-static tests. However, further efforts are required to model the dynamic influence, where the failure of the separator is predicted later than in the experiment.

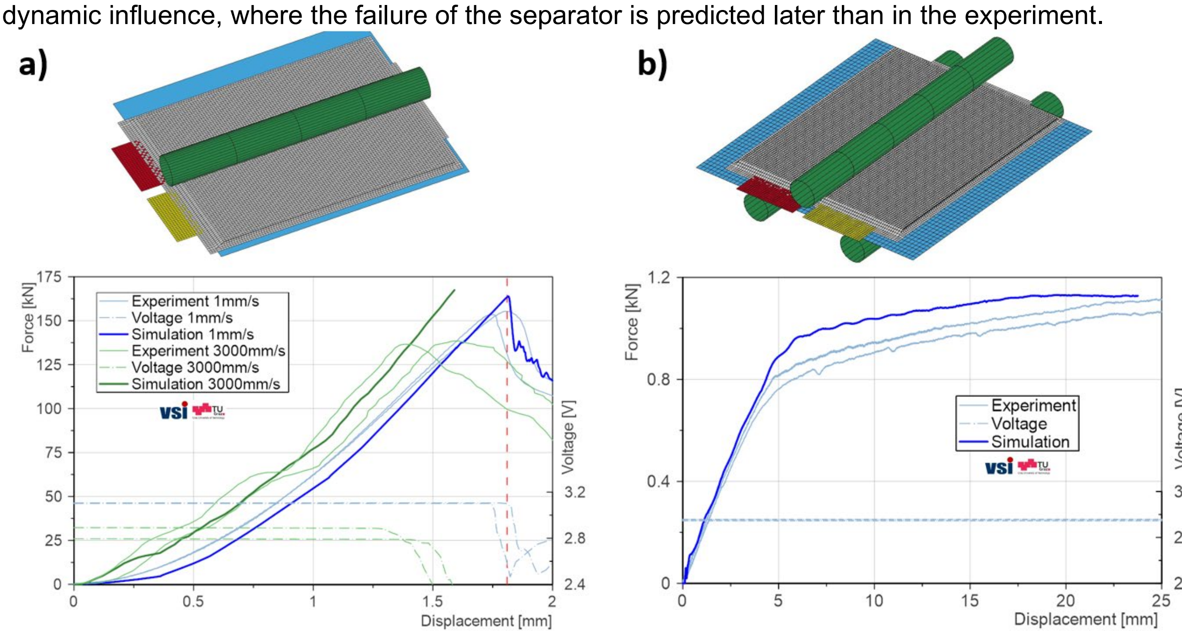

Fig.2: DLM results a: cylindrical indentation test - long side b: 3-Point bending test

On the right side, the results of the quasi-static 3-point bending test are shown. These data were used for the iterative adjustment of the interlaminar shear behaviour. The final detailed layer model of the pouch cell has an initial time step of 1.33E-05ms. The cell model consists of about 2.2 million nodes and 1.3 million elements (shell and solid). In our study, the cylindrical indentation test had a calculation duration of 48h (quasi-static) and 10h (dynamic) on a 64-core HPC cluster.

3 Simplified Applicable Model – SAM

In contrast to the Detailed Layer Model, the newly developed Simplified Applicable Model – SAM does not subdivide the jelly stack into the individual components. The entire jelly stack is considered a homogeneous system. The main advantage of this approach lies in the computational efficiency while accurately representing cell features like anisotropy and strain rate dependency at the same time.

Concept

To keep the computational effort low, this model mainly consists computationally efficient 1D and 2D elements (beam and shell). As shown in Fig. 3, the SAM approach can be divided into three main areas.

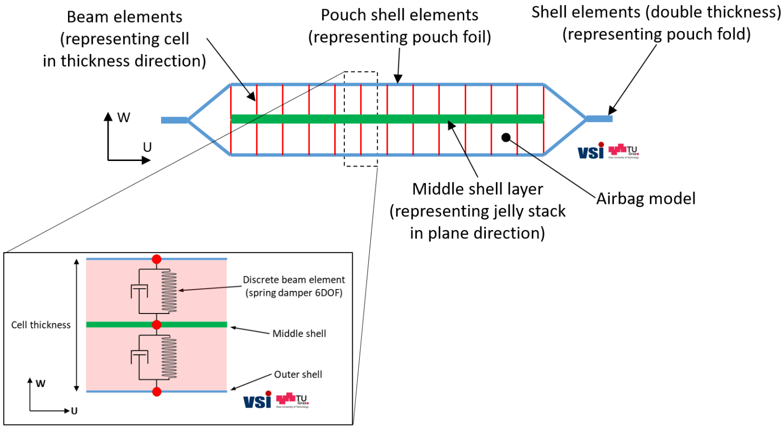

Fig.3: Concept of the Simplified Applicable Model

The first essential area is the middle layer. This represents the behaviour of the jelly stack in the in-plane direction. The discretisation is done by shell elements with a mesh size of 4x4mm. A fictitious tensile test of the entire jelly stack is used for the characterisation. Here, the same results of the component tests can be used as for the in-plane behaviour of the DLM. The results show that the influence of the separator on the behaviour of the jelly stack is negligible. Thus, it can be considered isotropic. The compression behaviour of the middle shell is characterised by the lateral indentation test, which is shown in Fig. 4 top. Since the results show that the tensile and compressive properties differ significantly, the material model ***MAT_PLASTICITY_COMPRESSION_TENSION** is used. This offers the possibility to define compression and tension behaviour separately. Such, the buckling of the struck-side layers (adjacent to the load head) is depicted in a simplistic way.

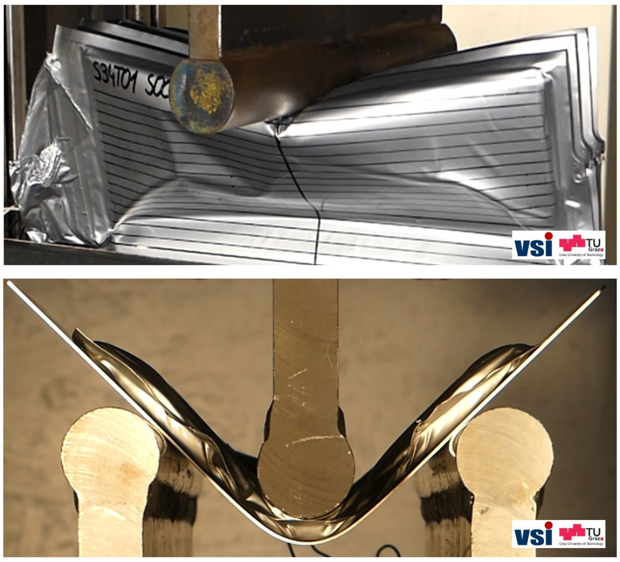

Fig.4: Top: Lateral indentation test Bottom: 3-Point bending test

The second area is the pouch envelope. Like the middle layer, it is discretised by shell elements. The tensile tests of the pouch material are used for the characterisation. Similar to the DLM model, the pouch is assumed to be isotropic. However, the yield stress in compression is modified to replicate the buckling, e.g. in bending loads (Fig. 4 bottom). Therefore, the material model ***MAT_PLASTICITY_COMPRESSION_TENSION** is employed. The volume of the pouch is controlled by using ***AIRBAG_LINEAR_FLUID**. Here, the electrolyte is again assumed incompressible, which means that the enclosed volume of the pouch does not change.

The last essential area comprises the elements that represent the cell behaviour in the thickness direction. Beam elements are used for the quasi-static behaviour. These connect the nodes of the middle layer with the nodes of the pouch. The material model used for this is ***GENERAL_NONLINEAR_6DOF_DISCRETE_BEAM**. The discrete elements ensure that the time step is independent of the element size and therefore not influenced by compression of the cell in the thickness direction. For the characterisation, the indentation test with cylindrical impactor is used. For the dynamic behaviour, solid elements are added (This was a work-around because adding damping to the discrete beams resulted in massive time-drops). These only have an effect at high compression rates. This means that these elements must only represent the difference between quasi-static and dynamic behaviour, since in the dynamic case both beams and solids are active. The material model used here is ***MAT_MODIFIED_HONEYCOMB**.
Due to the independent configuration of the model components, the behaviour in plane direction and transverse direction can be determined separately and thus the anisotropy of the cell can be taken into account. With the SAM approach, a generic short circuit criteria based on the beam element forces in the three principal directions was introduced.

3.1 Results

As with the DLM, the same selected load case are shown for SAM in comparison to the experimental results. (Fig. 5)

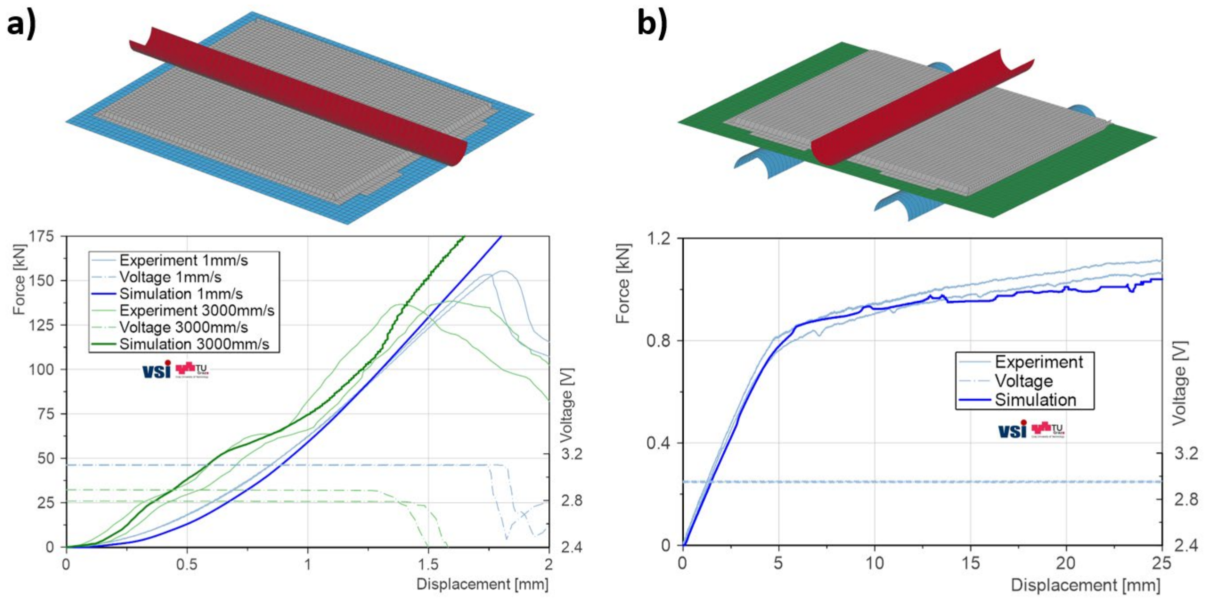

Fig.5: SAM results a) cylindrical indentation test - long side b) 3-Point bending test

As can be seen in Fig. 5a, both, the quasi-static and the dynamic behaviour in transverse compression and in 3-point bending, is replicated almost perfectly.
The macroscopic model presented here has about 15,000 nodes and 18,000 elements. The initial time step is 7.63E-4ms. In our investigations, this resulted in a computing duration of 2h (quasi-static) and 42sec. (dynamic) on an HPC cluster with 20 cores.

4 Summary

In this paper, two approaches for modelling lithium-ion pouch cells are presented. Only the mechanical behaviour is considered. The first approach (DLM) is a detailed consideration that distinguishes between the individual components. In this model, interlaminar contacts are not used. By using a fully decoupled material model assigned to the solid-elements between the shell-elements the transverse compression and interlaminar shear behaviour is replicated. This, in combination with a discrete element formulation, keeps the computational effort relatively low and increases the robustness of the model. For the characterisation, both, component tests and cell tests are required. From the latter, the behaviour in thickness direction and the bending behaviour are derived. The short-circuit prediction is done by simulating the component failure.

The second approach (SAM) is a macroscopic model. The computational effort is kept low by mainly using fast 1D and 2D elements (beams and shells). Several cell tests have been used for characterisation (or in fact calibration). The dynamic behaviour is generated by additional solid elements. These represent the difference between quasi-static and dynamic. The short-circuit prediction is based on the evaluation of beam-forces.

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