Development of a User-Defined Material Model for Sheet Molding Compounds

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Abstract. The compression molding of Sheet Molding Compounds (SMCs) is typically thought of as a fluid mechanics problem. The simulation of such materials is at present based on the background of compression or injection molded short fiber reinforced materials. The usage of CF-SMC consisting of high fiber volume content (over 50%) and long fiber reinforcement structures (up to 50 mm) challenges the feasibility of this point of view. The goal of this work is the development of a user-defined material model based on a solid mechanics formulation for SMC materials in LS-DYNA®. To allow for large deformations in the simulation an Arbitrary Lagrangian-Eulerian (ALE) approach is used. As a first step, a material characterization is carried out in a so-called press rheometer test where the mechanical behavior of the SMC material is analyzed during the compression molding process. The resulting stress response of the material then serves as input information for the material model. The material model itself is based on a modular building-block approach. The individual modules describe certain aspects of the material behavior (e.g. compaction, plastic flow behavior or fiber orientation) and interact with one another through the passing of parameters between the respective modules. This procedure allows for the flexible development of the mathematical description for each part of the material behavior. Initially, a simple mathematical model describes every module. In the further development of the model, each module is expanded by more complex mathematical descriptions. As the overall goal is a work in progress, this paper shows the current implementation of several of these modules including the characterized compression and flow behavior as well as a description for the fiber orientation based on the Folgar-Tucker equation. By simulating the press rheometer test itself using the developed user defined material model, a comparison between simulation and experiments is performed to check the accuracy of the various mathematical models used. The stress response and the flow front development provide the basis for the comparison and provide clues on how to proceed with the further development.

1 Introduction

The compression molding process allows the processing of complex and large part geometries made from Sheet Molding Compounds (SMC) including ribs and part inserts. The SMC material is a fiber-reinforced thermoset prepreg material with a typical fiber volume content between 15-60 weight-% of non-continues short or long glass, carbon or natural fibers (up to a length of 50 mm). In the compression molding process, pre-cut and stacked SMC material sheets are prepared at room temperature and then placed into a preheated mold and compressed by a hydraulic or mechanical press. During the pressing process the material is not only shaped and compacted, but also flows inside the mold to form the complex shape. [1]

Regarding the structural properties of an SMC component, the behavior which occurs during the pressing process is of crucial importance. This includes the final orientation of the reinforcing fibers, the positions of weld lines, local fiber volume content, as well as stresses and warpage of the component during curing and demolding. Therefore, process simulations are performed to predict these properties. A few specialized commercially available software tools can simulate the process in a 3D format. The simulation methods used in these software tools are typically based on a fluid mechanics formulation. Recently however, the use of carbon fiber based SMC materials (CF-SMCs) with high fiber volume contents (up to 50%) and very long carbon fibers (up to 50 mm long) has challenged this point of view. These materials have allowed manufacturing parts with much better structural properties than ordinary glass fiber and filler based SMC materials.

In [2] the main author has already presented a simulation method that uses the built-in possibilities available in LS-DYNA® to represent the compression molding process of SMC material. This method is based on the fluid-structure interaction capabilities in LS-DYNA® and allows large deformations of the SMC stack by using the Arbitrary Lagrangian-Eulerian (ALE) approach. However, during the development process, the method of just using already existing possibilities reaches its limit when it comes to correctly representing the complex material behavior of a CF-SMC material because of the non-existence of a suitable material model.
The main objective of this work is the development of a user-defined material model for SMC materials based on a solid mechanics formulation in LS-DYNA®. Due to the complex material behavior of a CF-SMC during the compression molding process, this material model is built on a building-block approach. Every block or module represents a certain aspect of the behavior and describes it using a simple mathematical formulation.
To develop an appropriate material model it is important to first characterize the material behavior in detail. Already at the beginning of the 1980s Silva-Nieto et al. carried out a rheological characterization of a GF-SMC material by using a parallel plate plastometer to analyze the squeeze-flow behavior [3]. In later years, squeeze-flow remained the focus of the characterization experiments for SMC materials. In more recent works, Dumont et al. analyzed the compressibility of SMC and took into account friction effects in a so-called compression rheometer [4]. Based on their experiments they also developed a FE simulation model [5].
These examples of previous works show the importance of correctly characterizing squeeze-flow behavior of SMC materials. With this in mind, material characterization tests on press rheometer equipment developed and designed at the IVW GmbH at different tool closing speeds were performed. The press rheometry data recorded during testing (more specifically the press force, tool closing position together with the tooling geometry and press setup) are all used to develop and verify a finite element characterization model, whereby the exact material characterization test carried out on the press rheometer is simulated.

2 Material characterization in a press rheometry test

The press rheometer is a practical test setup for compression molding in which a molding compound is pressed between two parallel tool plates. The closing of the tool initiates compaction and flow of the material. By measuring the normal force and the change in specimen height (tool plate distance) material properties, for example the stress vs. strain behavior or viscosity, can be deduced. Advantages of this test setup are simple specimen preparation and the transferability of the material behavior to the real compression molding process. [6]

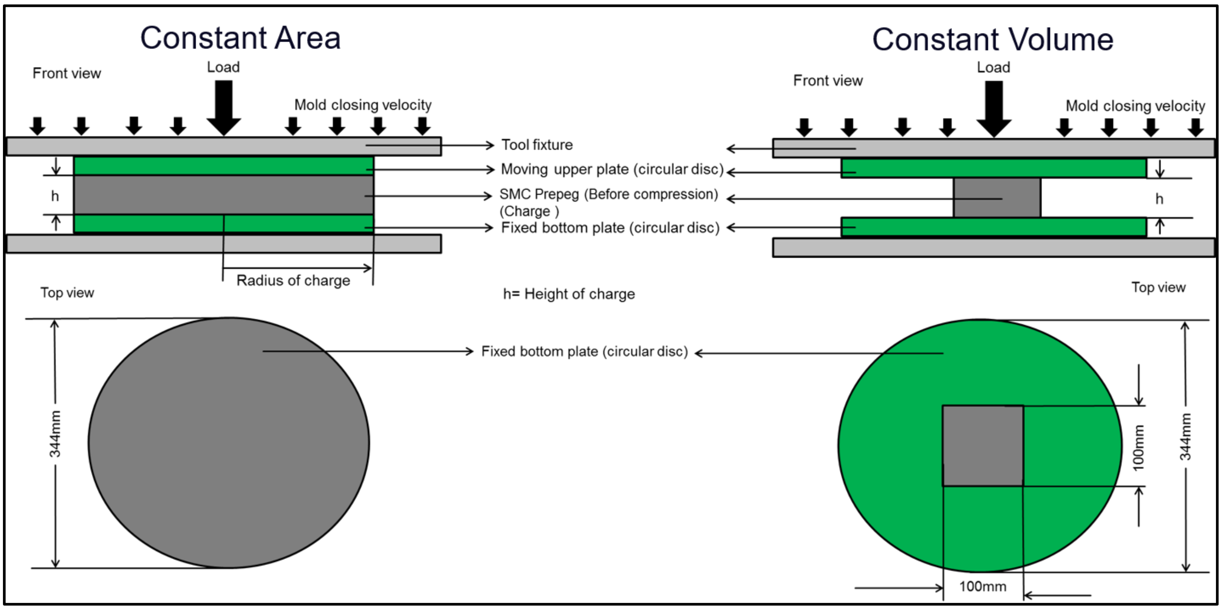

Fig. 1: Schematics of circular press rheometer setup for constant area (left) and constant volume (right) tests

In this work, a simple test setup with the open circular plate arrangement (Fig. 1) is used, where a material stack is placed in the middle of the plates and then flows out laterally unhindered when pressed.

The upper plate moves at a defined speed or force. This setup is based on the basic work of Lee et al. [7] and can be performed in two different configurations. A 100% full occupancy of the plate (constant area) allows an unhindered flow of the material and a clean force response regarding the flow behavior [2]. A smaller occupancy (constant volume) specimen size allows the analysis of the flow front development [8], the fiber orientation, as well as the homogeneity of the material.

Using the example of a commercially available CF-SMC material (Polynt Composites SMCarbon 24 CF50-12K) a typical result of a constant area test is shown in Fig. 2. The press data in the form of force and displacement information can be used to calculate the stress response of the SMC material during compression molding. The resulting effective stress versus effective strain curve can be divided into three areas. The detailed view, for smaller effective strain in Fig. 2 shows the first area where mainly compaction of the SMC stack takes place. In this phase, air pores, styrene and other gases are squeezed out of the material and the reinforcement structure is compacted. At this stage of pressing the SMC stack shows no in-plane flow behavior. After a certain level of compaction, the material begins an incompressible plastic flow phase and fills the cavity. At this stage the stress shows a linear behavior with only a small increase. At the end of the compression molding a fast increase in stress can be observed. Depending on the experimental setup this effect can have different reasons. In a real molding process it can be a sign for complete filling of the tool cavity. In the press rheometer setup considered here however, the material in this phase is almost completely pressed out and the tooling is almost completely closed which means a zero distance between the tool plates. The ratio between volume and surface of the specimen is so small that a plastic flow is no longer possible and the effective stress increases asymptotically.. In addition, for a very slow test velocity it is possible that the curing process begins which further increases the viscosity and slows down the plastic flow.

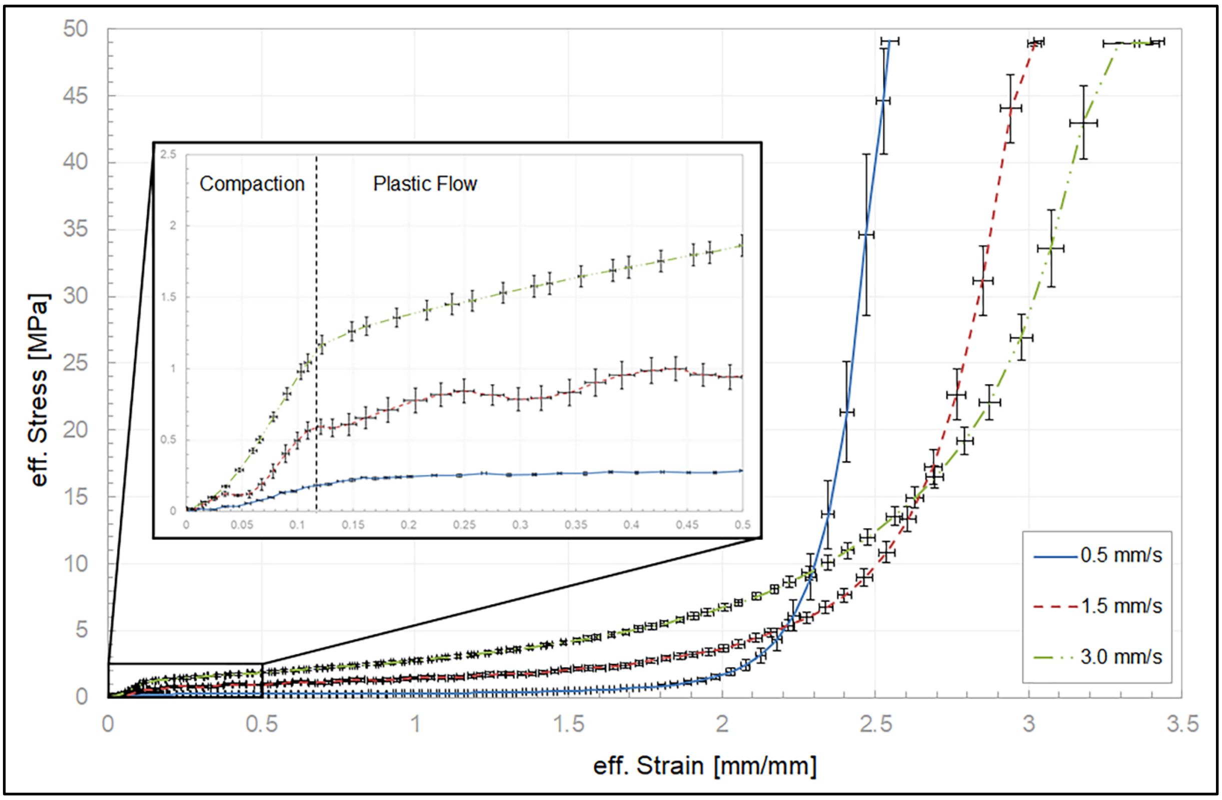

Fig. 2: Resulting stress response in constant area press rheometer test on SMCarbon 24 CF50-12K for different tool closing speeds

The difference in the curves for different tool closing speeds shows a strain rate dependency of the material. This strain rate dependency is a very important factor for a material model, however, the strain rate inside the material cannot be seen directly in these curves or in the test setup. In a circular press rheometer setup the strain rate depends on the radius (position of the considered volume). As an input parameter for a material model, an average strain rate would be sufficient. Fig. 3 shows a simple material independent way to determine the average strain rate. The slope of an effective strain versus experimental time curve describes the strain rate at a certain time (equivalent to the tool closing distance). All curves in this diagram can be separated and approximated by constant strain rate regions during the compaction and plastic flow phases of the experiment at the different tool closing velocities. The approximation therefore assumes the two phases can be described by linear trend lines which results in two different strain rates for each experiment.

While in the constant area test the material is always fully pressed out to a zero tool closing distance, the constant volume test is performed in short-shots with different tool closing distances of 3, 5, and 8 mm. The resulting flow fronts can directly be used for the verification of the material model as shown later in Fig. 9.

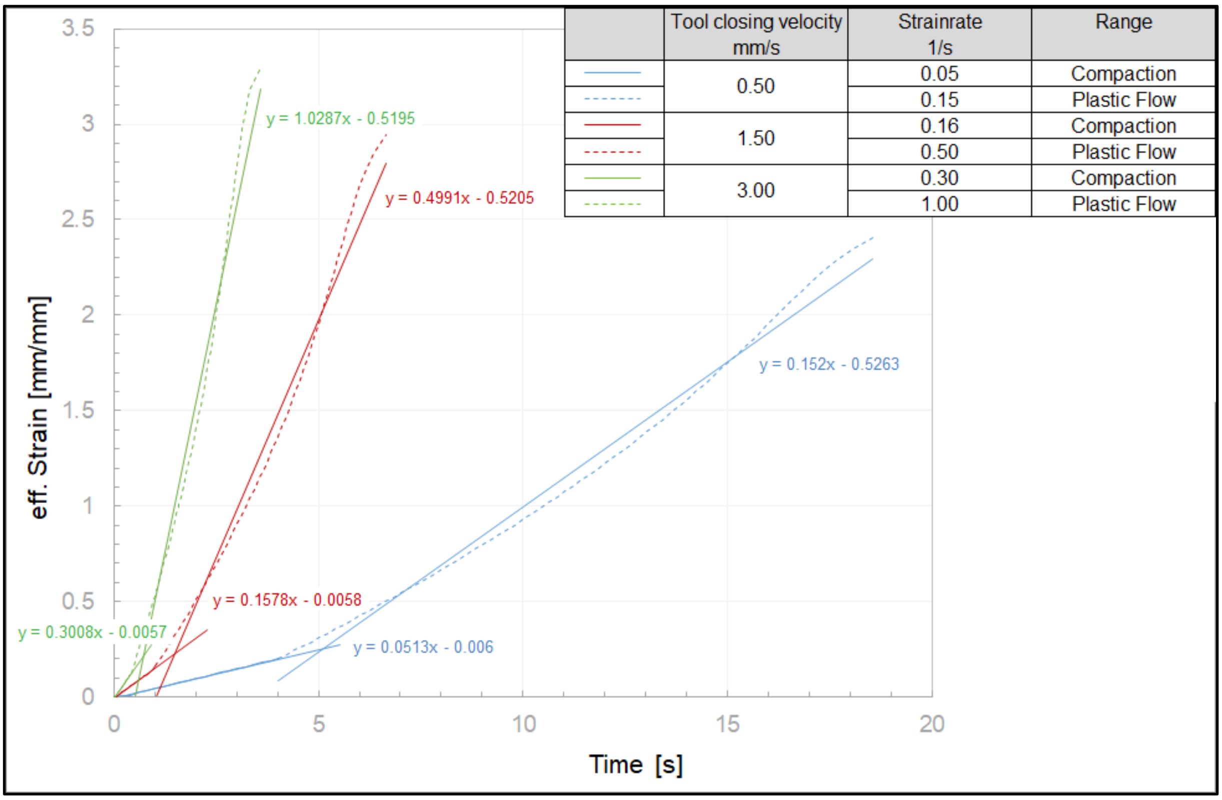

Fig. 3: Determination of the resulting average strain rate in the press rheometer test

3 Compression molding simulation in LS-DYNA®

During the compression molding process large distortions of the SMC material are expected because of the plastic flow behavior. This effect would cause large instabilities in a purely Lagrangian FEM formulation. To avoid these problems and to guarantee an accurate prediction of the material behavior the Arbitrary Lagrangian-Eulerian Method together with the Fluid- Structure Interaction (FSI) capabilities available in LS-DYNA® is chosen to simulate the compression molding process.

Based on the example of the press rheometer test, the setup of an ALE/FSI model is shown in Fig. 4. Because of the symmetry of the press rheometer, is the geometry has been simplified to a quarter model. For the definition of an ALE model it is necessary to model at least two volumes. These volumes work together as a single material and void or as in the present case ALE-multi-material-groups. Hereby, the fluid (SMC) volume can move inside the air (void) volume. In the ALE definition it is possible that the air volume can move or deform. In the present case this possibility is not appropriate, therefore the volume is constrained and defined as completely fixed. The defined fluid volume is the initial position of the SMC stack. Alternatively one can define the fluid volume in the keycard ***INITIAL_VOLUME_FRACTION_GEOMETRY** where the fluid and air together form a reference mesh.

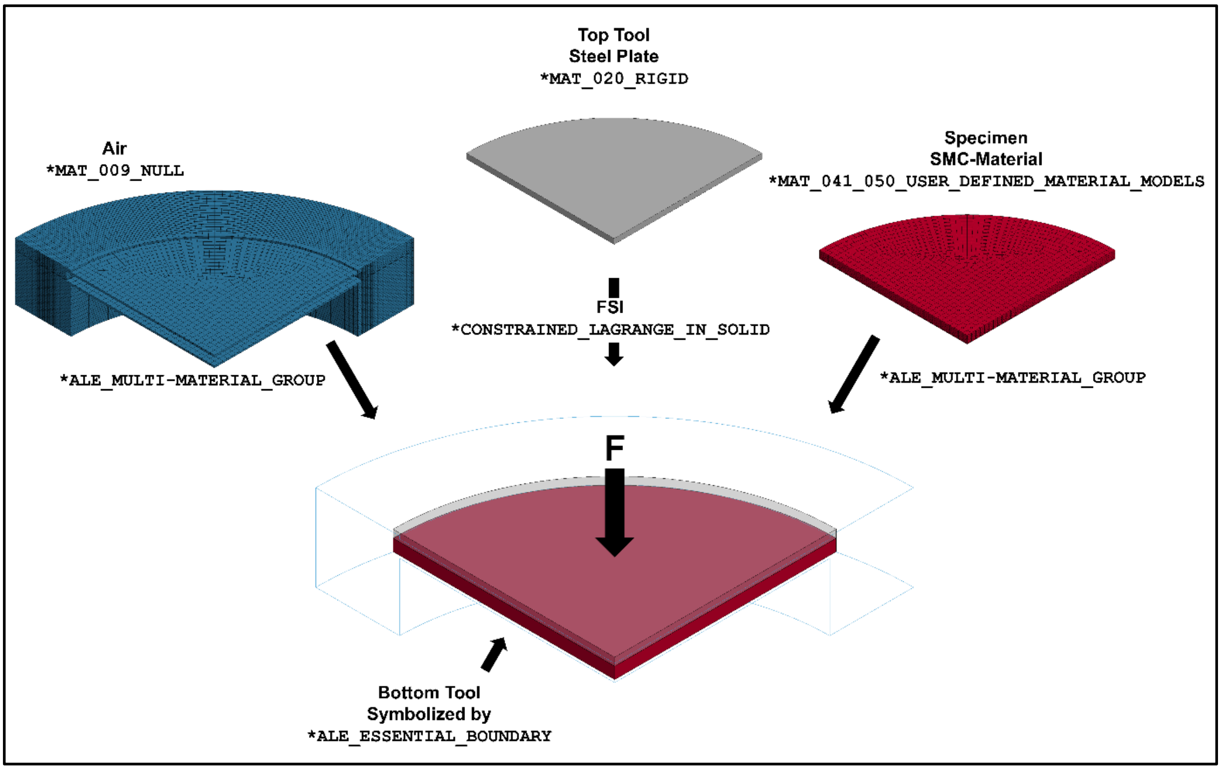

Fig. 4: ALE/FSI-Formulation of the press rheometry characterization test setup in LS-DYNA®

The calculation using the ALE method takes place in two steps. In a first Lagrangian step, stresses and strains are calculated within a Lagrangian formulation. After this, the new calculated parameters are remapped to the reference mesh. In this way it appears that the fluid material is flowing through the reference mesh as shown in Fig. 5. The tooling is defined as a Lagrangian body. The interaction between the ALE material and the Lagrangian body is defined by using the fluid-structure interaction capabilities available in LS-DYNA® in form of the ***CONSTRAINED_LAGRANGE_IN_SOLID** keycard. Because the bottom tool is not moving it has been omitted for simplification purposes. Instead an ***ALE_ESSENTIAL_BOUNDARY** condition is used to avoid movement of the fluid through the bottom side of the tool.

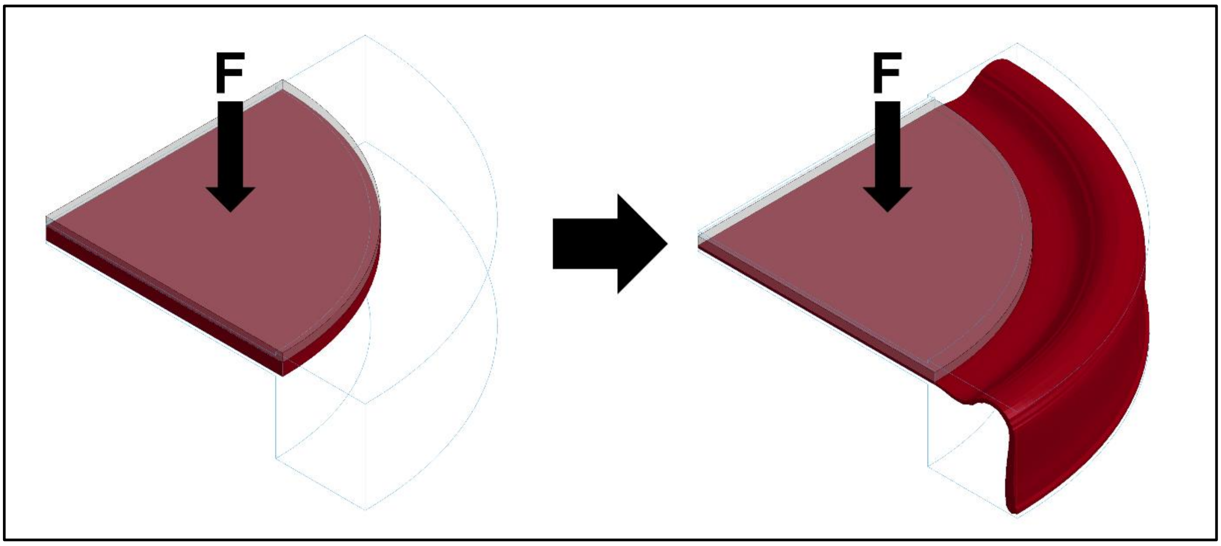

Fig. 5: Result of a compression molding simulation on the example of the press rheometer created in LS-DYNA®

4 User-defined material model for SMC

The user-defined material model is based on the principle of a building-block system (Fig. 6). Based on the result of the material characterization experiment, every block or module describes one characteristic of the material behavior using a simple mathematical model. Communication between the mathematical models takes place via the transfer of individual parameters between the modules. Following the implementation and validation of the individual modules, each module can be further developed and enhanced individually. As the development of the SMC material model is a work in progress, in this paper describes the already implemented parts of the model. The modules marked in grey are planned but have not yet been implemented at present.
Overall, the material model can be separated into a mechanical and a thermal part, although the thermal part has not yet been implemented. At present, it is also assumed that no curing effects occur in the very short time of a usual compression molding process. However, as the temperature will have an effect on the viscosity of the material during pressing (in other words the flow behavior) it is still considered as an important factor and will implemented at a later stage.

Instead of a module describing the compaction phase, a module called "Elasticity" can be seen in Fig. 6. This simplification is used for a first description of the compaction. In reality this part is not completely elastic. Due to squeeze out effects and rearrangement of the fiber reinforcement structure a complete recovery of the initial shape is not possible.

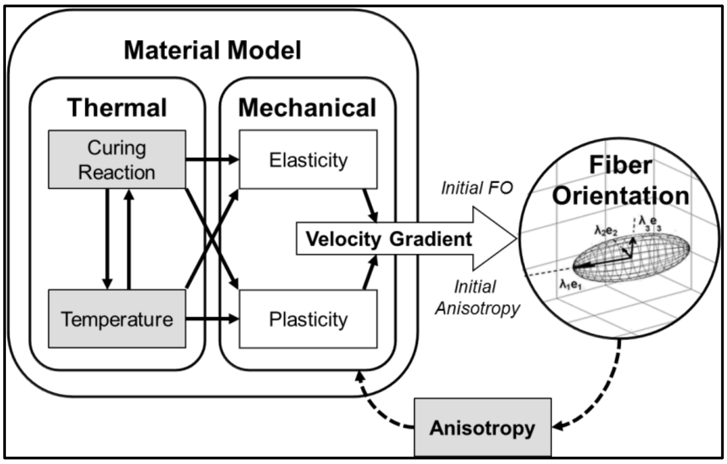

Fig. 6: Influencing factors and defined modules of the material model for Sheet Molding Compounds (SMC)

The elasticity in the model follows the Hooke's law and is taken from the example in the Appendix A of the LS-DYNA® manual [9]. This example is extended with a variable tensile modulus following a simple exponential correlation based on the effective strain ε_{eff} (Eq. 1). The parameters A and B are material constants.

$$E = A \cdot \exp(B \cdot \varepsilon_{eff}) \quad (1)$$

When reaching a certain yield stress, the behavior changes from a compressible elastic to an incompressible plastic description. Hereby is the plastic flow defined by a plasticity curve that describes the effective stress versus effective plastic strain. This plasticity curve can be deduced directly by the press rheometer (constant area type test) stress response curve. The definition of the plastic part by a curve allows also an implementation of the strain rate dependency by plotting plasticity curves for different speeds over the strain rate and then referencing them via a table. The corresponding stain rates can be found as was shown in Fig. 3.

One of the most interesting parameters when doing a process simulation with a fiber-reinforced material is the resulting fiber orientation. The fiber orientation is important for the structural behavior of the final component. Also during the compression molding itself, the evolution of the fiber orientation plays an important role in the compaction and flow behavior of the SMC material. The explicit modeling of individual fibers themself is out of the question as an accurate description will increase the calculation time immensely. Therefore it is important to implement a mathematical description into the material model. The first implementation of the calculation of the fiber orientation in the SMC material model developed here is based on a Folgar-Tucker equation (Eq. 2) that is classically used to describe injection molding processes of short fiber reinforced thermoplastic materials [10]. This equation describes the change over time t of a fiber orientation tensor A. M is here the Maier-Saupe Term (Eq. 3) which describes the influence of the velocity gradient ∇u and the geometry of the fibers with a geometry factor λ. The velocity gradient is also part of the shear strain tensor γ and the shear rate tensor $\dot{\gamma}$. The interaction between different fibers is described by the Folgar-Tucker diffusivity coefficient C_i.

$$\frac{DA}{Dt} = MA + AM^T - 2A{:}M - 6C_i\dot{\gamma}(A-\frac{1}{3}I) \tag{2}$$

$$M = \lambda\gamma + \frac{1}{2}(\nabla u-\nabla u^T) + \dot{\gamma}U_0A \tag{3}$$

5 Current results and discussion

With regards to the currently implemented modules of the material model, this first discussion of the results concentrates on the stress response of the simulation of the constant area press rheometer tests, the development of the flow front in the constant volume press rheometer tests as well as the plausibility of the predicted fiber orientation using the Folgar-Tucker equation.
Fig. 7 shows an overview of the main components of the fiber orientation tensor in a constant area test with a tool closing velocity of 0.5 mm/s. The resulting fiber orientation for the other velocities shows similar results. In the initial state, an in-plane isotropic fiber orientation with A11 and A22 equal to 0.5 and A33 equal to 0 was defined. It is remarkable that the orientation of the material that remains inside the tooling plates shows only a minor change in orientation. However, the material that flows to the outside changes significantly in terms of the fiber orientation. When the material leaves the tooling plates and begins to move under the influence of gravity in z-direction, we have a change in A33 that is not visible in the top view. Overall the fiber orientation prediction shows a plausible result. A more detailed analysis can be carried out when a demonstrator part with a more defined fiber orientation is available.

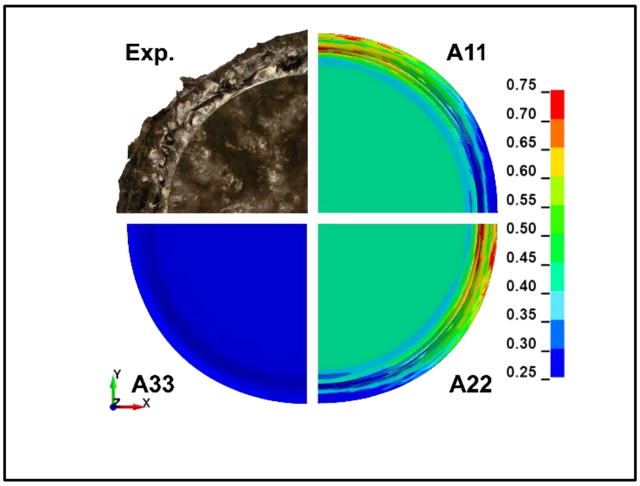

Fig. 7: Overview of the main components of the resulting fiber orientation tensor in a constant area press rheometer test simulation

The comparison of the stress response in a constant area press rheometer test between simulation and experiment shows a good approximation of the curves. It has to be mentioned that this result required a short calibration process of the input curve due to a lot of physical effects which are not taken into account in this first version of the material model. The stress response for a tool closing velocity of 0.5 mm/s cannot follow exactly the last part of the experimental curve. This is due to fact that in `*DEFINE_TABLE` overlapping curves are not allowed for interpolation reasons. The early increase of the experimental curve can also be explained by other influencing effects like a beginning curing of the material because of the slow pressing velocity (0.5 mm/s) of this experiment. The later implementation of curing effects in the material model is hope to alleviate this problem.

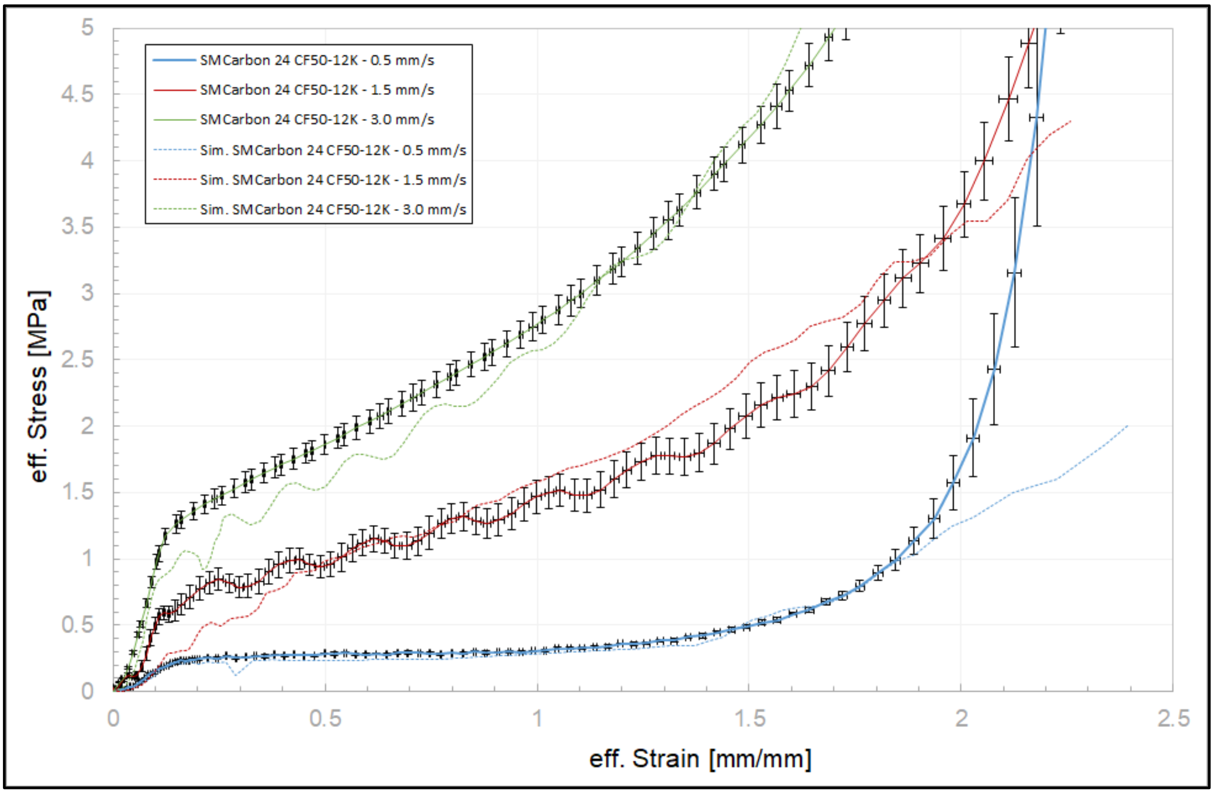

Fig. 8: Comparison between experiment and simulation with different tool closing velocities of 0.5, 1.5 and 3.0 mm/s

Fig. 9 shows the characterization results from a constant volume press rheometer test for decreasing plate-closing distances (so called short-shots). The white dashed square in the middle shows the initial stack size and position. The different markers represent the outlines of the average of three flow front experiments for each short-shot distance (3, 5, and 8 mm).

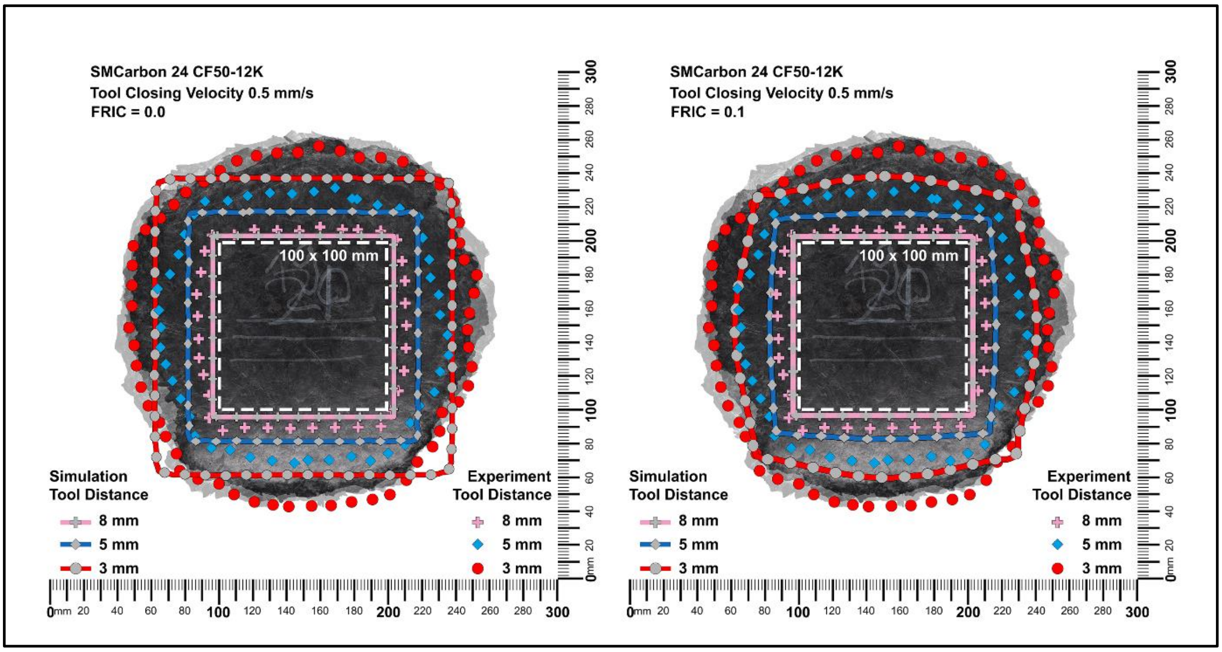

Fig. 9: Averaged flow front profiles for different tool closing distances during pressing at 0.5 mm/s and corresponding simulation results with a friction coefficient of 0 (left) and 0.1 (right)

The full lines represent the corresponding simulation results for comparison. In the direct comparison between simulation and experiment it can be seen that the experimental stack seems to flow further than in the simulation. An explanation for this effect can be found in the flow front behavior of the real material itself. In the experiment, it is observed that not all layers in the test specimen stack flow the same distance. For an individual specimen however, the outer most layer flow front contour is used to generate an averaged outer contour between several repeat specimens which is then used to make the comparison with the simulation. In the simulation, an average flow front distance based on the assumption of a block flow behavior is predicted (which will always be shorter than the average outer flow front contour) as no individual layers of the material are simulated.

In Fig. 9 (left), a simulation result without considering any friction effects is shown. Although the experimental stack shows the formation of a circular flow front shape, the simulation maintains a square shape because of its isotropic material definition. When considering friction, the simulated stack also begins to form a circular shape as can be seen in Fig. 9 (right). This means that friction between the tool and the specimen has a significant influence on the flow behavior of the SMC material. This effect has to be investigated in more detail in the future. Another influencing factor that will have an effect on the flow front shape is the anisotropy of the real material. Due to the existence of long fibers every SMC material shows a local anisotropy that has yet to be implemented into the model.

6 Conclusion

The actual simulation results show a good approximation of the real press rheometer material characterization experiments. Differences between the experiment and the simulation can be explained by missing physical and thermal effects which have yet to be implemented in the user defined material model. However, the most important factors have already been realized in the material model with intentionally simple models describing various aspects of the material behavior. The comparisons between experiment and simulation shown here leads to the next steps in the development process. The prediction of the flow front behavior can be further improved by the implementation of local material anisotropy effects and by considering the back coupling of the calculated fiber orientation tensor to the mechanical calculation. A further effect with significant influence is the friction between the tool and specimen. Here a closer investigation is necessary which should be carried out in parallel to the development of the material model.

7 Acknowledgement

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8 Literature

[1] Orgéas, L.; Dumont, P.; Nicolais, L.: Sheet Molding Compounds. In Wiley Encyclopedia Composites, 2012, 2683-2718.

[2] Schommer, D.; Duhovic, M.; Gortner, F; Maier, M.: Advanced Simulation of Polymer Composite SMC Compression Molding using Fluid-Structure Interaction in LS-DYNA®. 13th LS-DYNA User Conference, 2014, Dearborn, MI.

[3] Silva-Nieto, R. J.; Fisher, B. C.; Birley, A. W.: Rheological Characterization of Unsaturated Polyeseter Resin Sheet Molding Compound. Polymer Engineering and Science, Vol. 21, No. 8, 1981.

[4] Guiraud, O.; Dumont, P.J.J.; Orgéas, L.; Favier, D.: Rheometry of compression moulded fibre-reinforced polymer composites: Rheology, compressibility, and friction forces with mould surfaces. Composite: Part A, 43, 2012, 2107-2119.

[5] Dumont, P.; Orgéas, L.; Favier, D.; Pizette, P.; Venet, C.: Compression moulding of SMC: In situ experiments, modelling and simulation. Composite: Part A, 38, 2007, 353-368.

[6] Edelmann, K.: Prozeßintegrierte Analyse des Fließverhaltens von faserverstärkten thermoplastischen Preßmassen für die Serienfertigung. Dissertation, IVW Schriftenreihe, Band 18, 2001.

[7] Lee, L. J.; Marker, L. F.; Griffith, R. M.: The Rheology and Mold Flow of Polyester Sheet Molding Compound. Polymer Composites, Vol. 2, No. 4, 1981, 209-218.

[8] Barone, M. R.; Caulk, D. A.: Kinematics of Flow in Sheet Molding Compounds, Polymer Composites, Vol. 6, No. 2, 1985.

[9] N.N.: LS-DYNA® Keyword user’s manual. Volume I. LS-DYNA R9.0. 2016.

[10] Latz, A.; Strautins, U.; Niedziela, D.: Comparatitive numerical study of two concentrated fiber suspension models. Journal of Non-Newtonian Fluid Mechanics, 165, 2010, 764-781.