LICENTIATE THESIS

Towards 3D Modelling of Compression Moulding of SMC

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Fluid Mechanics

LULEÅ UNIVERSITY OF TECHNOLOGY

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Thesis for the degree: Teknologie Licensiat

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This thesis is dedicated to Henrik Kohkoinen. Rest in peace.

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Abstract

The automotive industry is facing ever increasing demands for reduced emissions, and lightweight solutions are thusly required. One field that has significant potential in this regard is composite materials, which can offer a good combination of weight reduction and mechanical properties. However, the rapid development cycles in the automotive industry mean that tools for numerical modeling are necessary, both regarding manufacturing processes and prediction of mechanical properties. The material that has been of interest for this work is Sheet Moulding Compound (SMC). SMC consists of sheets of resin and chopped fibres. When used for manufacturing the sheets are cut into appropriate size and shape. The cut sheets are then placed in a pre-heated mould. When this mould is closed, the sheets melt and the fibre-filled resin flows out and fills the mould cavity; the resin then cures and solidifies. A significant advantage of SMC compared to other composite solutions is that the process has comparatively short cycle times, which is a necessity for automotive applications. However, it is a rather complicated process to model numerically for a number of reasons, including the complex rheological properties of the charge, the often rather significant temperature gradients throughout the thickness, often complicated three-dimensional effects in the flow, and the chopped fibres present in the charge. These fibres will move and change orientation as the charge is pressed, which is a significant challenge to model properly. The first part of this work is a review and discussion of the difficulties described above, and some solutions that have been suggested. The second part concerns a suggestion for a three-dimensional flow model for the compression moulding process, which takes into account factors that have been suggested to influence the flow behavior, such as temperature distribution and shear strain rate. Some simulation results are presented along with comparison to previous experimental results, and similar flow patterns are observed serving as a qualitative validation. The third part concerns the expansion of this model to include the effects of the flow on the fibre orientation.

List of publications

Papers

Paper A : **Review of the Numerical Modeling of Compression Molding of Sheet Molding Compound**,
Gustaf Alnersson, M. Waseem Tahir, Anna-Lena Ljung and T. Staffan Lundström
MDPI Processes, Vol. 8, No. 2, 1-12,
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Paper B : **Numerical Study of The 3D-Flow Characteristics during Compression Moulding of SMC**,
Gustaf Alnersson, Anna-Lena Ljung and T. Staffan Lundström
Proceedings of the Twenty-Second International Conference on Composite Materials (ICCM22)

Paper C : **Fibre orientation for 3D-flow modelling of compression moulding of SMC**,
Gustaf Alnersson, Anna-Lena Ljung and T. Staffan Lundström
Manuscript

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Part I

Summary

Chapter 1

Introduction

The background to this PhD-project is that automotive vehicle parts are required to reduce their weight while at the same time improving their mechanical properties and having cost-effective manufacturing processes. Fibre reinforced polymer composites are generally light-weight high performance materials and have therefore been used in many applications including aerospace, sports, electrical insulations, and wind-turbines. This is therefore a class of materials that is likely to be increasingly used in vehicle manufacturing. Compared to, for instance, the aerospace industry, the vehicle industry does however brings even higher demands on cost-effective fast production meaning that several manufacturing methods of composites are too slow and costly, and are therefore not suitable. Compression moulding of Sheet Moulding Compound (SMC) is a process that has several advantages from an industrial standpoint; namely, that it is comparatively cheap (compared to other composite processes), that it is comparatively fast and that still relatively complex shapes can be produced. The process is typically used for products with moderate strength/stiffness to weight ratios, also within the vehicle industry. However, newly developed concepts may imply that SMC can be used also to manufacture high strength/stiffness to weight components. Hence ideally components manufactured with SMC may contribute to all three requirements of future vehicles, low weight, high performance and cost-effective fast manufacturing.

SMC consists of sheets made of a mixture of resin, chopped fibres and in some cases filling materials. The manufacturing process begins with cutting these sheets into desired shapes and sizes. These cut-outs are then placed inside a heated mould. The heat causes the cut-outs to melt as the tool is closed, which in turn leads to the material flowing out and filling the mould cavity. The mould is then held closed until the resin has cured, after which the part can be removed.

SMC is, however, associated with a number of issues, perhaps the most important one being that the quality of the finished product is greatly dependent on the parameters of the manufacturing, since the mechanical properties of the part are heavily dependent on how the fibres distribute and orient while the charge flows out in the mould. The flow is also rather difficult to model owing to the complicated rheological properties of the material, the high volume of solid materials, and the often quite significant temperature gradients through the thickness. These issues are discussed in greater detail in Paper A

The main research question for this project is "What are the mechanisms that govern flow during compression moulding of SMC?" This will be discussed in part in Chapter 2, after which the modelling of the flow is discussed in Chapter 3, while the modelling of the fibre orientations is the subject of Chapter 4. Finally some future work is discussed in Chapter 5.

Chapter 2

Experimental work

The experimental study of the rheological properties of SMC is complicated, mainly due to the presence of the fibres making the use of ordinary rheometers difficult. Significant early work was done by Barone and Caulk with regards to heat transfer and its consequences [1,2]; the flow was also studied using layers of SMC with different colours [3]. In these experiments it can be seen that a common feature of SMC flows is that the flow starts close to the upper and lower mould walls, and that the different layers can mix significantly in the parts of the cavity that are filled during the compression phase; this was also observed by Odenberger et al [4] who moulded SMC using an open mould and tracked the flow front using video cameras. Similar experiments to [3] were preformed by Olsson et al [5], with focus on finding ideal conditions for avoiding voids in the finalized parts. Perhaps most significantly to this work, the rheological properties of the SMC flow was investigated experimentally by Le Corre et al [6, 7] and by Dumont et al [8, 9], and several models for different aspects of the behaviour were suggested. An implementation of these models is further discussed in the "Flow Modelling" section as well as in Paper 2.

Chapter 3

Flow modelling

A number of early models were suggested by, among others, Silva-Nieto et al [10], Tucker and Folgar [11], Lee et al [12] and Barone and Caulk [13, 14]. These models share similarities in their assumptions regarding the flow as being essentially two-dimensional. The model most of interest here is the one proposed by Kluge et al [15]. It expands on the work by Marjavaara et al [16], whose model was in turn based on the semi-empirical relations suggested by Dumont et al [8, 9] and Le Corre et al [6, 7]. The model treats the combination of resin and fibres as a single medium, with a viscosity that depends on the temperature distribution, the shear strain rate and the volume fraction of fibres

$$\eta = 3\eta_0 \left(1 + 100 f_f + 1000 f_f^2\right) e^{-B\left(\frac{1}{T_0} - \frac{1}{T}\right)} \left(\frac{\dot{\varepsilon}}{\dot{\varepsilon}_0}\right)^{n-1} \left(1 + \dot{\gamma}^2\right)^{\frac{n-1}{2}}, \tag{1}$$

with f_f denoting the fibre volume fraction, B being a temperature constant, T denoting temperature, ε being related to how much the charge has been compressed compared to its initial thickness, γ denoting shear strain rate and the subscript 0 is used to mark initial conditions. It was also implemented by Kluge in order to attempt to predict pressure distributions inside mould, and their results aligned with experimental results.

Numerical results illustrating the dynamic viscosity retrieved with this model can be seen in Fig. 1. These results are discussed in further detail in Paper 2.

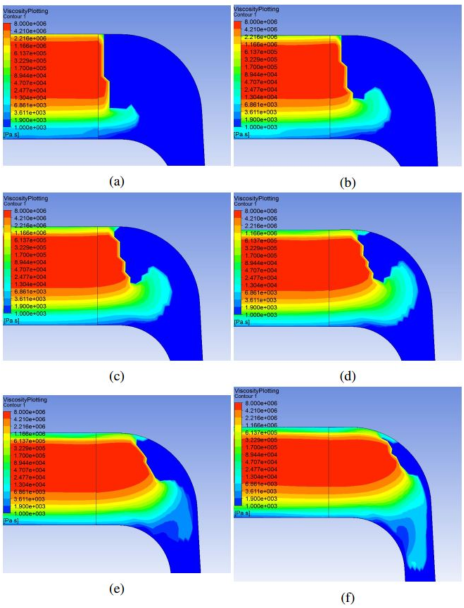

Figure 1: Examples of results of viscosity evolution during compression.

Chapter 4

Fibre modelling

The fibre orientation models used here are fundamentally based on the work of Jeffery [17], who built upon the work done by Einstein [18, 19] and derived the equations of motion for the case of an ellipsoidal particle in a viscous liquid. Folgar and Tucker [20] and Advani and Tucker [21] later built upon this and added a term, a so called rotary diffusion coefficient, that is meant to take into account the effects of particle-particle interactions without direct calculations. The resulting expressions for the time derivatives are thus

$$\frac{\mathrm{D}a_{ij}}{\mathrm{D}t} = -\frac{1}{2}\left(\omega_{ik}a_{kj} - a_{ik}\omega_{kj}\right) + \frac{1}{2}\lambda\left(\dot{\gamma}_{ik}a_{kj} + a_{ik}\dot{\gamma}_{kj} - 2\dot{\gamma}_{kl}a_{ijkl}\right) + 2D_r\left(\delta_{ij} - \alpha a_{ij}\right) \quad (2)$$

for the orientation tensors and

$$\dot{p}_i = -\frac{1}{2}\left(\omega_{ij}p_j\right) + \frac{1}{2}\lambda\left(\dot{\gamma}_{ij}p_j - \dot{\gamma}_{kl}p_k p_l p_i\right) - D_r\frac{1}{\psi}\frac{\propto \psi}{\propto \mathbf{p}}, \quad (3)$$

for the fibre angles. Here a_{ij} is the orientation tensor, ω is the vorticity, λ is a shape factor, γ is the shear strain rate, p is a unit vector that describes the fibre angles, ψ is the probability distribution function and D_r is the rotary diffusion coefficient, which depends on the shear and an experimentally determined constant.

Worth noting is that the model here presented is known to be flawed, especially with regards to underprediction of the alignment as a consequence of the strain rates in the flow [22]. A number of models exist to better take this into account [23, 24]; these are discussed in part in Paper A.

This model can then be combined with the flow modelling approach described in Section 3 to create a one-way coupling from the flow to the motions of the fibres. The averages of components of the orientation tensors can then be compared to experimental results, which can be seen in Table 1. The numerical results are well within the limits of the experimental results, and this is discussed in more detail in Paper 3.

Table 1: Experimental results from Advani and Tucker [25] compared to numerical results of the average values in the domain of the noted components of the orientation tensors. The numbers given in the left column indicate the percentage of the surface area of the mould that is covered by material at the start of pressing.

	a_{11}	a_{12}
Experimental (50)	0.624 ± 0.13	0.024 ± 0.008
Simulated (50)	0.520 ± 0.03	0.030 ± 0.01
Experimental (67)	0.594 ± 0.09	0.013 ± 0.01
Simulated (67)	0.560 ± 0.03	0.010 ± 0.008

Chapter 5

Future work

There are several approaches that could be taken regarding future work. One possible approach would be to simply build upon the existing framework and implement one of the more advanced forms of Advani-Tucker-based models, as seen in for instance Tseng et al [26] or Phelps and Tucker [27]. The approach taken here is simply to modify the rotary diffusion constant fron Eqs. (3) and (2) to better take interactions into account. Another possible approach is to implement some form of two-way coupling, i.e. the motions of the fibres are connected back to the solution of the flow [28, 29]. Yet another approach would be to use some form of Discrete Element Methods (DEM, see for instance [30]), either in some form of coupling with existing CFD models (i.e. DEM for the fibre motions), or for both the fluid and particle motions.

References

[1] M. R. Barone and D. A. Caulk, "The effect of deformation and thermoset cure on heat conduction in a chopped-fiber reinforced polyester during compression molding," *International Journal of Heat and Mass Transfer*, vol. 22, no. 7, pp. 1021–1032, 1979.

[2] M. R. Barone and D. A. Caulk, "Optimal Thermal Design of Compression Molds for Chopped-Fiber Composites," *Polymer Engineering and Science*, vol. 21, no. 17, pp. 1140—-1148, 1981.

[3] M. R. Barone and D. A. Caulk, "Kinematics of Flow in Sheet Molding Compounds," *Polymer Composites*, vol. 6, 1985.

[4] P. T. Odenberger, H. M. Andersson, and T. S. Lundström, "Experimental flow-front visualisation in compression moulding of SMC," *Composites Part A: Applied Science and Manufacturing*, vol. 35, no. 10, pp. 1125–1134, 2004.

[5] N. E. J. Olsson, T. S. Lundström, and K. Olofsson, "Design of experiment study of compression moulding of SMC," *Plastics, Rubber and Composites*, vol. 38, 2009.

[6] S. Le Corre, L. Orgéas, D. Favier, A. Tourabi, A. Maazouz, and C. Venet, "Shear and compression behaviour of sheet moulding compounds," *Composites Science and Technology*, vol. 62, no. 4, pp. 571–577, 2002.

[7] S. Le Corre, P. Dumont, L. Orgéas, and D. Favier, "Rheology of highly concentrated planar fiber suspensions," *Journal of Rheology*, vol. 49, no. 5, pp. 1029–1058, 2005.

[8] S. Le Corre, D. Favier, P. Dumont, and L. Orgéas, "Anisotropic viscous behavior of sheet molding compounds (SMC) during compression molding," *International Journal of Plasticity*, vol. 19, pp. 625–646, 2003.

[9] P. Dumont, L. Orgéas, D. Favier, P. Pizette, and C. Venet, "Compression moulding of SMC: In situ experiments, modelling and simulation," *Composites Part A: Applied Science and Manufacturing*, vol. 38, no. 2, pp. 353–368, 2007.

[10] R. J. SilvaNieto, B. C. Fisher, and A. W. Birley, "Predicting mold flow for unsaturated polyester resin sheet molding compounds," *Polymer Composites*, vol. 1, no. 1, pp. 14–23, 1980.

[11] C. L. Tucker and F. Folgar, "A model of compression mold filling," *Polymer Engineering & Science*, vol. 23, no. 2, pp. 69–73, 1983.

[12] C.-C. Lee, F. Folgar, and C. L. Tucker, "Simulation of Compression Molding for Fiber-Reinforced Thermosetting Polymers," *Journal of Engineering for Industry*, vol. 106, no. 2, p. 114, 1984.

[13] M. R. Barone and D. A. Caulk, "A Model for the Flow of a Chopped Fiber Reinforced Polymer Compound in Compression Molding," *Journal of Applied Mechanics*, vol. 53, no. 2, p. 361, 1986.

[14] M. R. Barone and T. A. Osswald, "A boundary element analysis of flow in sheet molding compound," *Polymer Composites*, vol. 9, no. 2, pp. 158–164, 1988.

[15] N. E. J. Kluge, T. S. Lundström, L. G. Westerberg, and K. Olofsson, "Compression moulding of sheet moulding compound: Modelling with computational fluid dynamics and validation," *Journal of Reinforced Plastics and Composites*, vol. 34, no. 6, pp. 479–492, 2015.

[16] B. D. Marjavaara, S. Ebermark, and T. S. Lundström, "Compression Moulding Simulations of SMC using a Multobjective Surrogate-based Inverse Modeling Approach," *Omega*, vol. 45, no. 5, pp. 503–514, 2009.

[17] G. B. Jeffery, "The Motion of Ellipsoidal Particles Immersed in a Viscous Fluid," *Proceedings of the Royal Society A*, pp. 161–179, 1922.

[18] A. Einstein, "Eine neue Bestimmung der Moleküldimensionen," *Annalen der Physik*, vol. 324, no. 2, pp. 289–306, 1906.

[19] A. Einstein, "Berichtigung zu meiner arbeit: 'eine neue bestimmung der molekuldimensionen," *Annalen der Physik*, vol. 34, pp. 591–592, 1911.

[20] F. Folgar and C. L. Tucker, "Orientation Behavior of Fibers in Concentrated Suspensions," *Journal of Reinforced Plastics and Composites*, vol. 3, no. 2, pp. 98–119, 1984.

[21] S. G. Advani and C. L. Tucker, "The Use of Tensors to Describe and Predict Fiber Orientation in Short Fiber Composites," *Journal of Rheology*, vol. 31, no. 8, pp. 751–784, 1987.

[22] M. Sepehr, P. J. Carreau, M. Moan, and G. Ausias, "Rheological properties of short fiber model suspensions," *Journal of Rheology*, vol. 48, no. 5, pp. 1023–1048, 2004.

[23] J. Wang, J. F. O'Gara, and C. L. Tucker, "An objective model for slow orientation kinetics in concentrated fiber suspensions: Theory and rheological evidence," *Journal of Rheology*, vol. 52, no. 5, pp. 1179–1200, 2008.

[24] H.-C. Tseng, R.-Y. Chang, and C.-H. Hsu, "Phenomenological improvements to predictive models of fiber orientation in concentrated suspensions," *Journal of Rheology*, vol. 57, no. 6, pp. 1597–1631, 2013.

[25] S. G. Advani and C. L. Tucker, “A numerical simulation of short fiber orientation in compression molding,” *Polymer Composites*, vol. 11, no. 3, pp. 164–173, 1990.

[26] H.-C. Tseng, R.-Y. Chang, and C.-H. Hsu, “An objective tensor to predict anisotropic fiber orientation in concentrated suspensions,” *Journal of Rheology*, vol. 60, pp. 215–224, 2016.

[27] J. H. Phelps and C. L. Tucker, “An anisotropic rotary diffusion model for fiber orientation in short- and long-fiber thermoplastics,” *Journal of Non-Newtonian Fluid Mechanics*, vol. 156, no. 3, pp. 165–176, 2009.

[28] G. G. Lipscomb, M. M. Denn, D. U. Hur, and D. V. Boger, “The flow of fiber suspensions in complex geometries,” *Journal of Non-Newtonian Fluid Mechanics*, vol. 26, no. 3, pp. 297–325, 1988.

[29] M. Maxey, “Simulation Methods for Particulate Flows and Concentrated Suspensions,” *Annual Review of Fluid Mechanics*, vol. 49, pp. 171–193, 2017.

[30] W. Zhong, A. Yu, X. Liu, Z. Tong, and H. Zhang, “DEM/CFD-DEM Modelling of Non-spherical Particulate Systems: Theoretical Developments and Applications,” *Powder Technology*, vol. 302, pp. 108–152, 2016.

Part II

Papers

Paper A

Review of the Numerical Modeling of Compression Molding of Sheet Molding Compound

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Review

Review of the Numerical Modeling of Compression Molding of Sheet Molding Compound

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Abstract: A review of the numerical modeling of the compression molding of the sheet molding compound (SMC) is presented. The focus of this review is the practical difficulties of modeling cases with high fiber content, an area in which there is relatively little documented work. In these cases, the prediction of the flows become intricate due to several reasons, mainly the complex rheology of the compound and large temperature gradients, but also the orientation of fibers and the micromechanics of the interactions between the fluid and the fibers play major roles. The details of this during moldings are discussed. Special attention is given to the impact on viscosity from the high fiber volume fraction, and the various models for this. One additional area of interest is the modeling of the fiber orientation.

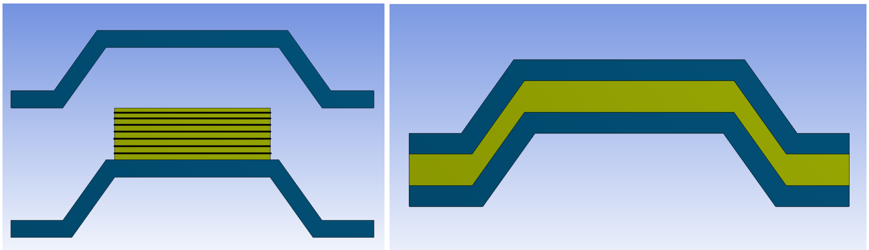
Keywords: sheet molding compound; compression molding; numerical modeling

1. Introduction

Fiber-reinforced polymer (FRP) composites are becoming increasingly attractive in areas where properties such as high strength, stiffness, and crash resistance are sought for as well as low weight, for instance in the automotive industry.

Glass or carbon fibers are often used as reinforcing materials. These fibers may be arranged in tows and weaved or stitched together to form fabrics. Different types of resins are used as matrices, including thermosets such as polyester, vinyl ester and epoxy, and thermoplastics such as nylon.

In the current review, the flow during compression molding of the sheet molding compound (SMC) is in focus. The main advantage with the compression molding of SMC is that the process is relatively fast as compared to many other processes to manufacture FRP composites and that the tooling is relatively cheap compared to metal forming [1]. Raw SMC material is also comparatively cheap compared to continuous fiber prepregs. SMC sheets are produced by spreading chopped fibers on a resin, which in most cases is a thermoset resin. The resin is then pressed between rollers to form sheets of SMC material. At room temperature, these sheets have a rubber-like appearance. A consequence of the random orientation of the chopped fibers in SMC is that the mechanical properties are not as good in comparison with continuous aligned fibers. However, if the fibers can be aligned in desired directions during the molding process, the mechanical properties can be improved extensively. For the process discussed here, pre-impregnated sheets of fibers and matrix are cut into parts of an appropriate size and placed inside a heated mold so that they cover an appropriate part of the tool, this can be seen in Figure 1. The mold is then closed so that the charge starts to flow and form the desired shape. The compression is then held for an appropriate time for the resin to be cured and the finished part can then be removed from the mold.



(**a**) Initial position. (**b**) Final position.

Figure 1. A schematic view of the process. (**a**) shows the open mold, with the charge between them and the black lines inside the charge showing the different layers. (**b**) then shows the final size, when the charge has fully filled the mold cavity.

One major issue with SMC parts, however, is that the quality of the finished parts is very sensitive to variations in the process parameters [2], which means that the properties may be difficult to predict with quality and trust. The chopped fibers that initially are orientated in, more or less, random directions may orientate during flow and the final part may get anisotropic mechanical properties as a result.

During the compression, the charge will flow inside the mold. The exact flow pattern will be determined by:

- The properties of the prefabricated charge
- The properties of the molten charge
- The geometry of the mold
- The placement of the charge
- The temperature of the charge and the mold
- The closing speed of the mold
- The tilting of the tools as they are closed

Hence numerical modeling of the molding process is complicated; the rheology of the molten compound is complex, there are significant temperature gradients, as well as three-dimensional effects in the flow front, and the geometries of the molds are often quite complex. There exist several commercial software packages, such as Autodesk Moldflow, Moldex3D and 3DTimon, that can be used to model the process. It should, however, be noted that all of the above were initially developed for injection molding, and there is not a significant amount of literature on the validation of these platforms with regards to compression molding of SMC [3].

Noteworthy early work on SMC was done by Barone and Caulk; including heat conduction in SMC [4,5], models of the flow [6,7], and experimental visualization of the flow [8]. Similar experiments have since been conducted by Olsson et al. [9]. An important conclusion drawn by Olsson et al. [9] is that a higher mold closing speed resulted in a more homogeneous flow, while a lower closing speed resulted in more mixing between the layers of the charge. Important early numerical work was performed by Tucker et al. [10] and Lee et al. [11], who developed a model for the flow of the charge based on Hele-Shaw flow (see for instance [12]). Significant work has also been done by Advani [13–16], especially with regards to the modeling of fiber orientation, and by Dumont and Le Corre, including both numerical modeling of fiber orientation [17,18] and experimental models of the rheology of SMC [19–23]. Some more recent efforts include Li et al. [3], Oter et al. [24], Song et al. [25], and Motaghi [26]. Several relatively new studies have also concerned the modeling of the entire process chain [27,28], concerning both process modeling [29,30] and mechanical modeling [31,32].

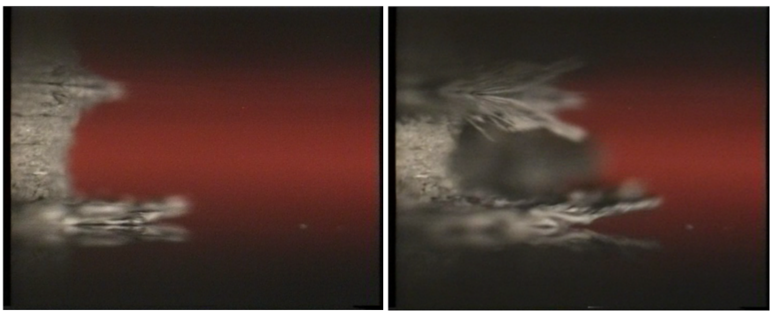
The focus of this review will be on the flow during the molding, meaning that aspects such as preparing of SMC or curing will not be considered.

The first step is a more detailed description of the compression molding process, Section 2. Section 3 then contains a more general description of the rheology during the molding, followed by a more in-depth discussion regarding viscosity modeling and fiber orientation in Sections 4 and 5 respectively. In Section 6 some additional newer initiatives involving interesting alternative methods for numerical simulation of the process are briefly discussed. Finally, Section 7 provides some concluding remarks.

2. Phenomenological Description of the Process

As briefly described above, during traditional compression molding of SMC, sheets of a rubber-like compound manufactured from a thermosetting resin, chopped fiber bundles, and possible some filler are loaded into a heated mold, the mold is closed and the charge will fill the mold. During this process, the compound is subjected to a mechanical load and heat. This will result in a pressure gradient and a temperature gradient within the compound. The temperature gradient will cause a gradient in viscosity while the pressure gradient will compress the compound (that is air pockets and voids) and initiates motion. Due to the large temperature and viscosity gradients, the flow will not be even, especially not at the start of the pressing. Instead, the compound located closest to the tooling will move first. This is shown in [33] for cases where stacks of 5 circular sheets with a diameter of 100 mm were placed between two parallel heated plates, after which the upper plate was set in motion towards the lower plate at a constant speed.

Different speeds and temperatures of the plates were used and the uneven flow was captured by video recordings of the flow front as shown in Figure 2 for a relatively low speed of 2 mm/s, an lower plate temperature of 135 °C and an upper plate temperature of 165 °C. It should be noted that the compound starts to flow near the lower plate as it had been subjected to heat for a longer time. This phenomenon was first observed by Barone [8] from partial moldings and later confirmed by molding using sheets of varying color by Olsson [9], where it is obvious that the outer layers end up at the flow front. Hence, the outer layers do not stay as outer layers which results in a complicated three-dimensional flow in the front of the SMC during pressing. From Figure 2 it can also be observed how the fibers with an averaged length of 26 mm seem to dominate the flow and there may be air entrapment at the flow front. Another observation in [33] is that due to the high temperatures the resin may start to boil in areas with low pressures creating voids. For an open mold as the one presented in [33], this will happen at the flow front, while for a closed mold it may still happen that the pressure from the compression does not reach all areas within the mold. This may, for instance, be due to the geometry of the mold, partly cured resin, or that the fibers carry the load.



(**a**) (**b**)

Figure 2. Flow front progression for a relatively low speed of 2 mm/s, a lower plate temperature of 135 °C and an upper plate temperature of 165 °C [33]. The charge bulk of fibers and resin can be seen as the gray area in the left image (**a**). It can be seen that the flow starts closer to the mold walls before the bulk starts to move (**b**). These are previously unpublished photos.

In addition to boiling there are often also voids in the compound; air may be entrapped between the layers of the compound during lay-up and air may be entrapped at the flow front during compression, see Figure 2. Larger amounts of voids may influence the pressure build-up, the viscosity distribution and the flow of the compound. The transport of voids during compression was studied by Sentis [34] using 3D synchrotron X-ray for compounds with weight fiber contents of 29% and 50%. It was shown that the initial volume void contents of 1.5%–5.5% and 23% for the respective cases were reduced to nearly zero during the compression. Two mechanisms for the removal of the voids were observed: a transport out of the compound as described in detail in [35,36], and a dissolution into the resin as also discussed in [37,38] for liquid molding processes. To exemplify by using model materials and Particle Image Velocimetry Westerberg [36] show that voids may move faster than the suspension towards the fluid flow front during pressing.

The geometry of the mold is another important aspect of the compression molding of SMC. To exemplify the manufactured parts are often designed with stiffeners such as ribs of different shapes; to make the compound with relatively long fiber bundles flow into these can be challenging.

3. Rheological Measurements of SMC

The rheology of the SMC during the molding process is complicated for a number of reasons, among them are:

- High fiber content
- The relatively long fibers
- The orientation of the fibers
- The fibers are flexible
- Air is displaced
- Variations in the material
- Anisotropic viscosity

Most of these points (1–4) will be discussed in Sections 4 and 5. Displacement of air and material variations can mostly be considered as things that should be avoided rather than measured or modeled. Anisotropic viscosity is mainly a result of the fiber orientation, this will be discussed briefly in Section 4. Integrated "black-box" values of rheological properties of the SMC may, however, also be captured from experiments, although a significant issue is that ordinary rheometers usually cannot be used due to the long fibers. Some early experimental studies were conducted by Lee et al. [39]. The viscous properties of glass fiber SMC were studied for varying temperatures and average fiber lengths. A simple model for the viscosity of SMC between two parallel plates was suggested

$$\eta_e \simeq \left[\frac{1}{6} \left(\frac{L}{H} \right)^2 \frac{V_f}{1 - V_f} \right] \eta \quad (1)$$

with L as the length of the plates, H the separation between them, V_f being the volume fraction of fibers and η the basic viscosity of the medium. The authors however stated that this model would probably not be valid for more complex charges and molds.

Vahlund and Gebart [40] used a modified press that allowed measurement of rheology in large tools; by using a set of pressure sensors the pressure in the charge was measured for a range of closing speeds ranging from 3 to 30 mm/s and a similarly wide range of press forces. Le Corre et al. [21] also developed a rheometer in a larger scale to be able to properly measure the properties, the results of this will be discussed in Section 4.

A rheological aspect which has more recently been suggested by experiments by Ferré-Sentis et al. [34,41] is that considering the SMC charge as incompressible might be an unrealistic assumption. This is likely connected to air both inside the sheets and between them. Hohberg et al. [29]

did similar experiments as Ferré-Sentis and developed a model for how a compressible SMC affects its rheological properties, with reasonably good agreement with experimental results.

4. Models for the Viscosity

A vast amount of research has been carried out on the relations between solid fraction in suspension and viscosity, see [42–45] for instance. To exemplify Einstein [46,47] and later Batchelor and co-authors in a series of papers [48–51] developed models from first principles that are useable for low fractions of monodispersed particles. Einsteins model, for instance, may be written as

$$\eta_{susp} = \eta\,(1 + 2.5\phi) \tag{2}$$

while the Batchelors model, assuming a Brownian suspension in a Newtonian liquid, can be written as

$$\eta_{susp} = \eta\left(1 + 2.5\phi + 6.2\phi^2\right) \tag{3}$$

In both these expressions, ϕ is the volume fraction of particles and it is assumed that the suspension is dilute. For larger solid fractions empirical models have been derived, for example from Ferrini et al. [52].

Work on the extensional viscosity of semi-dilute suspensions of elongated particles was also presented by Batchelor [53], Dihn and Armstrong [54], and Acrivos and Shaqfeh [55].

However, these models become problematic when dealing with prolonged particles. One reason is that the number of possible contacts between particles generally increases with the aspect ratio of particles [56,57] and that orientation and torque of the particles become important factors [58,59].

Several semi-empirical relations for how various factors affect the viscosity of the SMC charge have also been suggested. It was found by Le Corre et al. [21] that the viscosity mainly depends on three factors: strain rate, temperature and fiber volume fraction. The dependence on the strain rate can be described using a Carreau viscosity model as established by Lee et al. [39]

$$\eta = \eta_0\left(1 + (\lambda\dot{\gamma})^2\right)^{\frac{n-1}{2}} \tag{4}$$

where λ is a time constant, $\dot{\gamma}$ is the shear rate, and n is a power-law index.

Dependence on fiber volume fraction and temperature was also studied experimentally by Le Corre et al. [21] and Dumont et al. [19,20]. They suggested that the fiber fraction dependence could be described as

$$\eta = 3 \cdot \eta_{paste}\left(\frac{\dot{\epsilon}}{\dot{\epsilon}_0}\right)^{n-1}\left(1 + 100 \cdot f_f + 1000 \cdot f_f^2\right) \tag{5}$$

where the subscript 0 indicates initial conditions, η_{Paste} is the temperature-dependent viscosity, f_f is the fiber volume fraction, $\dot{\epsilon}$ is the strain rate and n is a power law index. The temperature dependence was described as

$$\eta_{paste} = \eta_0 e^{-b\left(\frac{1}{T_0} - \frac{1}{T}\right)} \tag{6}$$

in which η_0 is the initial viscosity of the charge and T is the temperature. A model based on Equation (6) was implemented numerically in Marjavaara et al. [60] and expanded with Equations (4) and (5) in Kluge et al. [61]. In both these works, the goal was to numerically determine the pressure field, and those models were then compared to experimental data with relatively good agreement.

A subject that has been discussed is whether the viscosity model should take into account differences between the bulk of the flow and the layers closest to the mold walls. Kluge et al. [61], for instance, evaluated a number of different models with different formulations both with the same equation for viscosity through the charge and with a separate equation for the viscosity of the skin closest to the walls and for the cases studied it was concluded that a one equation model was sufficient to predict the pressure in the mold.

More recently a model was suggested by Bertóti and Böhlke [62], in which the viscosity of the flow was shown to be affected by the orientation of the fibers. A viscosity tensor was introduced that takes into account the fiber orientation, the shape of the charge and the material properties of the charge. The fiber orientation was modeled using the orientation model suggested by Advani and Tucker [13]. This new viscosity model does not consider temperature, fiber volume fraction or curing; however, the authors outline the procedure to include this.

Favaloro et al. [63] also studied the connection between viscosity and fiber orientation and derived an expression for a term referred to as Informed Isotropic Viscosity

$$\eta_{IISO} = \eta_m \kappa_{23} \left[1 + 4 \left(R_\eta - 1 \right) \left(\frac{D_r}{\dot{\gamma}} : A : \frac{D_r}{\dot{\gamma}} \right) \right] \tag{7}$$

where η_m is the viscosity of the matrix, κ_{23} is a factor connecting shear to viscosity, R_η is a term describing the anisotropy of the viscosity (that will be equal to 1 for an isotropic viscosity), and $\dot{\gamma}$ is the magnitude of the strain rate. A and D_r are the fiber orientation tensor and a tensor connected to the evolution of fiber orientation respectively, both of these terms will be discussed further in Section 5. Tseng and Favaloro [64] implemented Equation (7) for injection molding procedures and obtained good agreement with experimental results.

5. Modeling of Fiber Orientation

Most of the work relating to the modeling of fiber orientation in the compression molding of SMC is based on the work of Jeffery [65]. Jeffery extended Einstein's work [46,47] and derived expressions for the motion of a single ellipsoidal particle immersed in a fluid by solving the equations of motion.

Folgar and Tucker [66] adapted Jeffery's work specifically for fibers in concentrated suspensions. This was done by adding a term, called a rotary diffusion term, to account for the interaction between the fibers. A problem with their initial model, however, is that it involves the probability distribution function (PDF) of the angles of the fibers, which is a more realistic case results in a prohibitively expensive computational load.

Advani and Tucker [13] suggested a solution to this problem by representing the PDF as a set of tensors, which results in an expression for the motion of a single fiber

$$\dot{p}_i = -\frac{1}{2} \left(\omega_{ij} p_j \right) + \frac{1}{2} \lambda \left(\dot{\gamma}_{ij} p_j - \dot{\gamma}_{kl} p_k p_l p_i \right) - D_r \frac{1}{\psi} \frac{\propto \psi}{\propto p} \tag{8}$$

and the equation

$$\frac{\mathrm{D} a_{ij}}{\mathrm{D} t} = -\frac{1}{2} \left(\omega_{ik} a_{kj} - a_{ik} \omega_{kj} \right) + \frac{1}{2} \lambda \left(\dot{\gamma}_{ik} a_{kj} + a_{ik} \dot{\gamma}_{kj} - 2 \dot{\gamma}_{kl} a_{ijkl} \right) + 2 D_r \left(\delta_{ij} - \alpha a_{ij} \right) \tag{9}$$

for the evolution of the second-order orientation tensor, where ω is the vorticity tensor, $\dot{\gamma}$ is the strain rate tensor, a_{ij} is the second-order orientation tensor, λ is a parameter describing the shape of the particle, p is a unit vector describing the orientation of a fiber with p_i being functions of the fiber angles, ψ is the PDF, $\frac{\propto \psi}{\propto \mathbf{p}}$ is the gradient operator on the surface of the unit sphere created by p, δ_{ij} is the Kronecker delta, and α is a constant connected to whether planar or three-dimensional orientation is calculated. D_r is the previously mentioned rotary diffusion term, which in the case suggested by Folgar and Tucker [66] depends on the shear rate and the constant C_I, which is called the interaction coefficient. The value of C_I must usually be determined by experiments and by letting C_I vary it is possible to adapt Equation (8) to many different cases. The approach in [13] results in equations that do not have a closed form as an orientation tensor of the higher-order will appear in every term describing the change of the orientation tensor. A closure approximation, i.e., a way to approximate the equations in a closed form, is thus required; this can be done in a variety of ways [15].

One important difference between the Advani model (Equation (8)) and experimental results is that the fibers align more slowly than the model predicts [67,68]. Several amendments to this model have therefore been suggested. Wang et al. [67] suggested the Reduced Strain Closure (RSC) model, in which the diffusion term is multiplied by a constant term κ, and the closure approximation is modified by a term depending on κ and the current fiber angles. In the case where κ is equal to 1, Equation (8) is recovered. An alternative approach was suggested by Phelps and Tucker [69], which they labeled the ARD–RSC (Anisotropic Rotary Diffusion–Reduced Strain Closure). They suggested that Hand's tensor [70] could be used to connect the diffusion closer to the fiber orientation. To do this five experimental parameters are required. According to Tseng et al. [71], this may result in issues with the numerical stability of the obtained solutions. They thus formulated their own model, called iARD–RPR (Improved Anisotropic Rotary Diffusion–Retardant Principal Rate), which has four constants and fewer terms overall than the ARD–RSC model; however, a critical issue with this formulation is that it is dependent on the coordinate frame used. Tseng et al corrected this issue in a later paper [72]. Worth noting is that parameters in all these models might not be readily accessible in more realistic cases.

A common theme among these fiber orientation models is that they are phenomenological, which means that they might be very good for specific processes to which they have been tuned, but not necessarily good for a more general case. Another common problem is that they are based on an assumption of Newtonian flow which as previously mentioned is a somewhat unrealistic assumption. Dumont et al. [17] numerically studied fiber evolution using both Jeffery and Folgar–Tucker with various different closure approximations, as well as a more direct method for directly modeling the fiber–fiber interactions. They found that the model that best modeled the fiber motion in a more general case is the Jeffery equation; it was also stated that the tested phenomenological models did not perform well in more general cases.

Another detail is that the fibers tend to be regarded either as rigid ellipsoids or as rigid rods, while in reality they can be bent, both during the manufacturing of the sheets and because of the flow during molding. One method has been suggested is the Beam–Rod model [73–75], where each fiber is modeled as two rigid segments connected by a bead. This formulation is then used to extend the Folgar–Tucker approach. Another similar possible method for addressing this issue is Direct Fiber Simulation suggested by Schmid [76] and Lindström [77] where the fibers are also modeled using the rod and bead formulation. The difference is that this method does not involve the Folgar–Tucker based method involving the PDF.

An alternative model has been suggested [78,79] where the fiber network is modeled as a deformable porous media. There is some work done regarding this with regards to injection molding processes (see for instance [80]), but to the authors best knowledge this has not been successfully applied to compression molding of discontinuous fibers.

6. Possible Areas of Future Research

There are several areas of research that are of interest, especially with regards to the issue of fiber orientation since this is arguably the greatest challenge associated with numerical modeling.

The previously mentioned method where the fiber network is modeled as a deformable porous medium might be an interesting alternative to the traditional fiber orientation models. Another method was proposed by Oter et al. [24], where lubrication theory is used to describe the flow, and the fiber orientation is described without using equations based on Jeffery's equation. This has still only been used for a two-dimensional problem, but suggestions were made for generalizing their method to more complex geometries. Yet another was presented by Schommer et al. [81], who described the charge using an Arbitrary Lagrangian–Eulerian formulation. Another possible method is Discrete

Element Modeling (DEM) (see for instance [82]). By modeling the fibers as composite particles, i.e., built as sequences of lesser particles, both fiber bending and breakage could be modeled.

An associated issue with any model, suggested above or otherwise, is that models should also preferably be applicable in an industrial context, which imposes limits on the complexity and time consumption. Connected to this is the issue of predicting the mechanical properties of the finalized SMC parts. This will not be discussed in detail in this paper, but the approach of Görthofer et al. [27] allowed the mapping between results of compression molding simulations into structural models with good accuracy regarding predictions of structural properties. Until new models for the fiber orientation have been developed a possible route forward is to use commercial software as those presented in the introduction and calibrate them with experiments.

7. Concluding Remarks

A review regarding the practical difficulties of numerical modeling of the compression molding of SMC has been presented. Several key issues such as modeling of fiber orientation and modeling of viscosity have been discussed, as well as approaches for dealing with these issues. One conclusion that can be drawn is that there is yet room for significant future work. This is especially true with regard to the numerical modeling of fiber orientation.

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Abbreviations

The following abbreviations are used in this manuscript:

SMC	Sheet molding compound
FRP	Fiber-reinforced polymer

References

1. Åström, B.T. *Manufacturing of Polymer Composites*, 1st ed.; Chapman & Hall: London, UK, 1997.
2. Martulli, L.M.; Muyshondt, L.; Kerschbaum, M.; Pimenta, S.; Lomov, S.V.; Swolfs, Y. Carbon fibre sheet moulding compounds with high in-mould flow: Linking morphology to tensile and compressive properties. *Compos. Part A Appl. Sci. Manuf.* **2019**, *126*, 105600, doi:10.1016/j.compositesa.2019.105600.
3. Li, Y.; Chen, Z.; Xu, H.; Dahl, J.; Zeng, D.; Mirdamadi, M.; Su, X. Modeling and Simulation of Compression Molding Process for Sheet Molding Compound (SMC) of Carbon FIber Composites. *SAE Int. J. Mater. Manuf.* **2017**, *10*, 130–137.
4. Barone, M.R.; Caulk, D.A. The effect of deformation and thermoset cure on heat conduction in a chopped-fiber reinforced polyester during compression molding. *Int. J. Heat Mass Transf.* **1979**, *22*, 1021–1032, doi:10.1016/0017-9310(79)90175-3.
5. Barone, M.R.; Caulk, D.A. Optimal Thermal Design of Compression Molds for Chopped-Fiber Composites. *Polym. Eng. Sci.* **1981**, *21*, 1140–1148.
6. Barone, M.R.; Caulk, D.A. A Model for the Flow of a Chopped Fiber Reinforced Polymer Compound in Compression Molding. *J. Appl. Mech.* **1986**, *53*, 361, doi:10.1115/1.3171765.
7. Barone, M.R.; Osswald, T.A. A boundary element analysis of flow in sheet molding compound. *Polym. Compos.* **1988**, *9*, 158–164, doi:10.1002/pc.750090210.
8. Barone, M.R.; Caulk, D.A. Kinematics of Flow in Sheet Molding Compounds. *Polym. Compos.* **1985**, *6*, 105–109.

9. Olsson, N.E.J.; Lundström, T.S.; Olofsson, K. Design of experiment study of compression moulding of SMC. *Plast. Rubber Compos.* **2009**, *38*, 426–431.
10. Tucker, C.L.; Folgar, F. A model of compression mold filling. *Polym. Eng. Sci.* **1983**, *23*, 69–73, doi:10.1002/pen.760230204.
11. Lee, C.C.; Folgar, F.; Tucker, C.L. Simulation of Compression Molding for Fiber-Reinforced Thermosetting Polymers. *J. Eng. Ind.* **1984**, *106*, 114, doi:10.1115/1.3185921.
12. Batchelor, G.K. *An Introdution to Fluid Mechanics*; Cambridge University Press: Cambridge, UK, 1967; pp. 216–228.
13. Advani, S.G.; Tucker, C.L. The Use of Tensors to Describe and Predict Fiber Orientation in Short Fiber Composites. *J. Rheol.* **1987**, *31*, 751–784, doi:10.1122/1.549945.
14. Advani, S.G.; Tucker, C.L. A numerical simulation of short fiber orientation in compression molding. *Polym. Compos.* **1990**, *11*, 164–173, doi:10.1002/pc.750110305.
15. Advani, S.G.; Tucker, C.L. Closure approximations for three-dimensional structure tensors. *J. Rheol.* **1990**, *34*, 367–386, doi:10.1122/1.550133.
16. Advani, S.G. *Flow and Rheology in Polymer Composites Manufacturing*; Elsevier: Amsterdam, The Netherlands, 1994.
17. Dumont, P.J.; Le Corre, S.; Orgéas, L.; Favier, D. A numerical analysis of the evolution of bundle orientation in concentrated fibre-bundle suspensions. *J. Non-Newton. Fluid Mech.* **2009**, *160*, 76–92, doi:10.1016/j.jnnfm.2009.03.001.
18. Dumont, P.J.J.; Le Corre, S.; Orgéas, L.; Favier, D.; Gaborit, C.; Lory, P. Finite Element Implementation of a Two-Phase Model for Compression Molding of Composites. *Eur. J. Comput. Mech.* **2005**, *14*, 883–900.
19. Dumont, P.; Orgéas, L.; Favier, D.; Pizette, P.; Venet, C. Compression moulding of SMC: In situ experiments, modelling and simulation. *Compos. Part A Appl. Sci. Manuf.* **2007**, *38*, 353–368, doi:10.1016/j.compositesa.2006.03.010.
20. Le Corre, S.; Favier, D.; Dumont, P.; Orgéas, L. Anisotropic viscous behavior of sheet molding compounds (SMC) during compression molding. *Int. J. Plast.* **2003**, *19*, 625–646.
21. Le Corre, S.; Orgéas, L.; Favier, D.; Tourabi, A.; Maazouz, A.; Venet, C. Shear and compression behaviour of sheet moulding compounds. *Compos. Sci. Technol.* **2002**, *62*, 571–577, doi:10.1016/S0266-3538(01)00151-8.
22. Le Corre, S.; Dumont, P.; Orgéas, L.; Favier, D. Rheology of highly concentrated planar fiber suspensions. *J. Rheol.* **2005**, *49*, 1029–1058, doi:10.1122/1.1993594.
23. 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. *Compos. Part A Appl. Sci. Manuf.* **2012**, *43*, 2107–2119, doi:10.1016/j.compositesa.2012.06.006.
24. Oter, L.; Abisset-Chavanne, E.; Chinesta, F.; Keunings, R.; Binetruy, C.; Comas-Cardona, S.; Perez, M.; Aufrere, C. A step towards the numerical simulation of SMC compression moulding. In *AIP Conference Proceedings*; AIP Publishing LLC: Melville, NY, USA, 2016.
25. Song, Y.; Gandhi, U.; Sekito, T.; Vaidya, U.; Hsu, J.; Yang, A.; Osswald, T. A Novel CAE Method for Compression Molding Simulation of Carbon Fiber-Reinforced Thermoplastic Composite Sheet Materials. *J. Compos. Sci.* **2018**, *2*, 33, doi:10.3390/jcs2020033.
26. Motaghi, A. Direct Sheet Molding Compound Process (D-SMC). Ph.D. Thesis, The University of Western Ontario, London, ON, Canada, 2018.
27. Görthofer, J.; Meyer, N.; Pallicity, T.D.; Schöttl, L.; Trauth, A.; Schemmann, M.; Hohberg, M.; Pinter, P.; Elsner, P.; Henning, F.; et al. Virtual process chain of sheet molding compound: Development, validation and perspectives. *Compos. Part B Eng.* **2019**, *169*, 133–147, doi:10.1016/j.compositesb.2019.04.001.
28. Hohberg, M. Experimental Investigation and Process Simulation of the Compression Molding Process of Sheet Molding Compound (SMC) with Local Reinforcements. Ph.D. Thesis, Karlsruher Instituts für Technologie, Karlsruhe, Germany, 2018.
29. Hohberg, M.; Kärger, L.; Henning, F.; Hrymak, A. Rheological measurements and rheological shell model Considering the compressible behavior of long fiber reinforced sheet molding compound (SMC). *Compos. Part A Appl. Sci. Manuf.* **2017**, *95*, 110–117, doi:10.1016/j.compositesa.2017.01.006.
30. Hohberg, M.; Kärger, L.; Henning, F.; Hrymak, A. Comparison of the flow and rheological behavior of two semi-structural Sheet-Molding-Compound (SMC) based on a hybrid resin and glass or carbon fibers. In *AIP Conference Proceedings*; AIP Publishing LLC: Melville, NY, USA, 2019; Volume 2139, doi:10.1063/1.5121660.

31. Görthofer, J.; Schemmann, M.; Seelig, T.; Hrymak, A.; Böhlke, T. Sensitivity Analysis of Fiber-Matrix Interface Parameters in an SMC Composite Damage Model. *Proceedings* **2018**, *2*, 544, doi:10.3390/icem18-05438.
32. Schemmann, M.; Görthofer, J.; Seelig, T.; Hrymak, A.; Böhlke, T. Anisotropic meanfield modeling of debonding and matrix damage in SMC composites. *Compos. Sci. Technol.* **2018**, *161*, 143–158, doi:10.1016/j.compscitech.2018.03.041.
33. Odenberger, P.T.; Andersson, H.M.; Lundström, T.S. Experimental flow-front visualisation in compression moulding of SMC. *Compos. Part A Appl. Sci. Manuf.* **2004**, *35*, 1125–1134, doi:10.1016/j.compositesa.2004.03.019.
34. Ferré Sentis, D.; Orgéas, L.; Dumont, P.J.; Rolland du Roscoat, S.; Sager, M.; Latil, P. 3D in situ observations of the compressibility and pore transport in Sheet Moulding Compounds during the early stages of compression moulding. *Compos. Part A Appl. Sci. Manuf.* **2017**, *92*, 51–61, doi:10.1016/j.compositesa.2016.10.031.
35. Lundstöm, T.S. Bubble Transport Through Constricted Capillary Tubes With Application to Resin Transfer Molding. *Polym. Compos.* **1996**, *17*, 770–779.
36. Westerberg, L.G.; Lundström, T.S.; Olsson, N.E.J. Transport of Bubbles During Compression in a Non-Newtonian Fluid. In Proceedings of the ITP2009: Interdisciplinary Transport Phenomena VI: Fluid, Thermal, Biological, Materials and Space Sciences, Volterra, Italy, 4–9 October 2009; pp. 10–22.
37. Lundström, T.S. Measurement of void collapse during resin transfer moulding. *Compos. Part A Appl. Sci. Manuf.* **1997**, *28*, 201–214, doi:10.1016/S1359-835X(96)00109-1.
38. Lundström, T.S.; Holmgren, A. Dissolution of voids during compression molding of SMC. *J. Reinf. Plast. Compos.* **2010**, *29*, 1826–1837, doi:10.1177/0731684409336369.
39. Lee, L.J.; Marker, L.F.; Griffith, R.M. The rheology and mold flow of polyester sheet molding compound. *Polym. Compos.* **1981**, *2*, 209–218, doi:10.1002/pc.750020412.
40. Vahlund, C.F.; Gebart, B.R. Squeeze Flow Rheology in Large Tools. In Proceedings of the 5th International Conference on Flow Processes in Composite Materials, Plymouth, UK, 12–14 July 1999; pp. 365–372.
41. Ferré Sentis, D.; Cochereau, T.; Orgéas, L.; Dumont, P.J.; Rolland du Roscoat, S.; Laurencin, T.; Terrien, M.; Sager, M. Tensile behaviour of uncured sheet moulding compounds: Rheology and flow-induced microstructures. *Compos. Part A Appl. Sci. Manuf.* **2017**, *101*, 459–470, doi:10.1016/j.compositesa.2017.07.003.
42. Chang, C.; Powell, R.L. Effect of particle size distributions on the rheology of concentrated bimodal suspensions. *J. Rheol.* **1994**, *38*, 85–98, doi:10.1122/1.550497.
43. Stickel, J.J.; Powell, R.L. Fluid Mechanics and Rheology of Dense Suspensions. *Annu. Rev. Fluid Mech.* **2005**, *37*, 129–149, doi:10.1146/annurev.fluid.36.050802.122132.
44. Maxey, M. Simulation Methods for Particulate Flows and Concentrated Suspensions. *Annu. Rev. Fluid Mech.* **2017**, *49*, 171–193, doi:10.1146/annurev-fluid-122414-034408.
45. Morris, J.F. Shear Thickening of Concentrated Suspensions: Recent Developments and Relation to Other Phenomena. *Annu. Rev. Fluid Mech.* **2020**, *52*, doi:10.1146/annurev-fluid-010816-060128.
46. Einstein, A. Eine neue Bestimmung der Moleküldimensionen. *Ann. Phys.* **1906**, *324*, 289–306, doi:10.1002/andp.19063240204.
47. Einstein, A. Berichtigung zu meiner Arbeit: 'Eine neue Bestimmung der Molekuldimensionen. *Ann. Phys.* **1911**, *34*, 591–592.
48. Batchelor, G.K.; Green, J.T. Determination of the bulk stress in a suspension of spherical particles to order c2. *J. Fluid Mech.* **1972**, *56*, 401–427.
49. Batchelor, G.K.; Green, J.T. The hydrodynamic interaction of two small freely-moving spheres in a linear flow field. *J. Fluid Mech.* **1972**, *56*, 375–400, doi:10.1017/S0022112072002927.
50. Batchelor, G.K. Brownian diffusion of particles with hydrodynamic interaction. *J. Fluid Mech.* **1976**, *74*, 1–29, doi:10.1017/S0022112076001663.
51. Batchelor, G.K. The effect of Brownian motion on the bulk stress in a suspension of spherical particles. *J. Fluid Mech.* **1977**, *83*, 97–117, doi:10.1017/S0022112077001062.
52. Ferrini, F.; Ercolani, D.; de Cindio, B.; Nicodemo, L.; Nicolais, L.; Ranaudo, S. Shear viscosity of settling suspensions. *Rheol. Acta* **1979**, *18*, 289–296, doi:10.1007/BF01542776.
53. Batchelor, G.K. The stress generated in a non-dilute suspension of elongated particles by pure straining motion. *J. Fluid Mech.* **1971**, *46*, 813–829, doi:10.1017/S0022112071000879.
54. Dinh, S.M.; Armstrong, R.C. Rheological equation of state for semi-concentrated fibre suspensions. *J. Rheol.* **1984**, *207*, doi:10.1122/1.549748.

55. Acrivos, A.; Shaqfeh, E.S.G. The effective thermal conductivity and elongational viscosity of a nondilute suspension of aligned slender rods. *Phys. Fluids* **1988**, *31*, 1841, doi:10.1063/1.866681.
56. Toll, S. Note: On the tube model for fiber suspensions. *J. Rheol.* **1993**, *37*, 123–125, doi:10.1122/1.550460.
57. Toll, S. Packing mechanics of fiber reinforcements. *Polym. Eng. Sci.* **1998**, *38*, 1337–1350, doi:10.1002/pen.10304.
58. Högberg, S.M.; Åkerstedt, H.O.; Lundström, T.S.; Freund, J.B. Respiratory deposition of fibers in the non-inertial regimedevelopment and application of a semi-analytical model. *Aerosol Sci. Technol.* **2010**, *44*, 847–860, doi:10.1080/02786826.2010.498455.
59. Holmstedt, E.; Åkerstedt, H.O.; Lundström, T.S. Modelling transport and deposition of non-spherical micro- and nano-particles in composites manufacturing. *J. Reinf. Plast. Compos.* **2018**, *37*, 507–519, doi:10.1177/0731684417753741.
60. Marjavaara, B.D.; Ebermark, S.; Lundström, T.S. Compression Moulding Simulations of SMC using a Multobjective Surrogate-based Inverse Modeling Approach. *Omega* **2009**, *45*, 503–514.
61. Kluge, N.E.J.; Lundström, T.S.; Westerberg, L.G.; Olofsson, K. Compression moulding of sheet moulding compound: Modelling with computational fluid dynamics and validation. *J. Reinf. Plast. Compos.* **2015**, *34*, 479–492, doi:10.1177/0731684415573981.
62. Bertóti, R.; Böhlke, T. Flow-induced anisotropic viscosity in short FRPs. *Mech. Adv. Mater. Mod. Process.* **2017**, *3*, 1.
63. Favaloro, A.J.; Tseng, H.C.; Pipes, R.B. A new anisotropic viscous constitutive model for composites molding simulation. *Compos. Part A Appl. Sci. Manuf.* **2018**, *115*, 112–122, doi:10.1016/j.compositesa.2018.09.022.
64. Tseng, H.C.; Favaloro, A.J. The use of informed isotropic constitutive equation to simulate anisotropic rheological behaviors in fiber suspensions. *J. Rheol.* **2019**, *63*, 263–274, doi:10.1122/1.5064727.
65. Jeffery, G.B. The Motion of Ellipsoidal Particles Immersed in a Viscous Fluid. *Proc. R. Soc. A* **1922**, *102*, 161–179.
66. Folgar, F.; Tucker, C.L. Orientation Behavior of Fibers in Concentrated Suspensions. *J. Reinf. Plast. Compos.* **1984**, *3*, 98–119, doi:10.1177/073168448400300201.
67. Wang, J.; O'Gara, J.F.; Tucker, C.L. An objective model for slow orientation kinetics in concentrated fiber suspensions: Theory and rheological evidence. *J. Rheol.* **2008**, *52*, 1179–1200, doi:10.1122/1.2946437.
68. Sepehr, M.; Carreau, P.J.; Moan, M.; Ausias, G. Rheological properties of short fiber model suspensions. *J. Rheol.* **2004**, *48*, 1023–1048, doi:10.1122/1.1773783.
69. Phelps, J.H.; Tucker, C.L. An anisotropic rotary diffusion model for fiber orientation in short- and long-fiber thermoplastics. *J. Non-Fluid Mech.* **2009**, *156*, 165–176, doi:10.1016/j.jnnfm.2008.08.002.
70. Hand, G.L. A theory of anisotropic fluids. *J. Fluid Mech.* **1962**, *13*, 33–46, doi:10.1017/S0022112062000476.
71. Tseng, H.C.; Chang, R.Y.; Hsu, C.H. Phenomenological improvements to predictive models of fiber orientation in concentrated suspensions. *J. Rheol.* **2013**, *57*, 1597–1631, doi:10.1122/1.4821038.
72. Tseng, H.C.; Chang, R.Y.; Hsu, C.H. An objective tensor to predict anisotropic fiber orientation in concentrated suspensions. *J. Rheol.* **2016**, *60*, 215–224.
73. Strautins, U.; Latz, A. Flow-driven orientation dynamics of semiflexible fiber systems. *Rheol. Acta* **2007**, *46*, 1057–1064, doi:10.1007/s00397-007-0194-7.
74. Ortman, K.C.; Velez, G.M.; Eberle, A.P.; Baird, D.G.; Wapperom, P. Long glass fiber orientation in thermoplastic composites using a model that accounts for the flexibility of the fibers. In Proceedings of the Annual Technical Conference–ANTEC, Chicago, IL, USA, 22–24 June 2009; Volume 1, pp. 585–589.
75. Ortman, K.; Baird, D.; Wapperom, P.; Aning, A. Prediction of Fiber Orientation in the Injection Molding of Long Fiber Suspensions Kevin. *Polym. Compos.* **2012**, *33*, 136–1367.
76. Schmid, C.F.; Switzer, L.H.; Klingenberg, D.J. Simulations of fiber flocculation: Effects of fiber properties and interfiber friction. *J. Rheol.* **2000**, *44*, 781–809, doi:10.1122/1.551116.
77. Lindström, S.B.; Uesaka, T. Simulation of the motion of flexible fibers in viscous fluid flow. *Phys. Fluids* **2007**, *19*, doi:10.1063/1.2778937.
78. Hellström, J.G.I.; Frishfelds, V.; Lundström, T.S. Mechanisms of flow-induced deformation of porous media. *J. Fluid Mech.* **2010**, *664*, 220–237, doi:10.1017/S002211201000368X.
79. Lundström, T.S.; Hellström, J.G.I.; Frishfelds, V. Transversal flow-induced deformation of fibres during composites manufacturing and the effect on permeability. *J. Reinf. Plast. Compos.* **2013**, *32*, 1129–1135, doi:10.1177/0731684413491846.

80. Ambrosi, D.; Preziosi, L. Modeling injection molding processes with deformable porous preforms. *Siam J. Appl. Math.* **2000**, *61*, 22–42, doi:10.1137/S0036139998333671.
81. Schommer, D.; Duhovic, M.; Gortner, F.; Maier, M. Advanced Simulation of Polymer Composite SMC Compression Molding using Fluid-Structure Interaction. In Proceedings of the 13th International LS-DYNA Users Conference, Detroit, MN, USA, 8–10 June 2014; pp. 1–10.
82. Zhong, W.; Yu, A.; Liu, X.; Tong, Z.; Zhang, H. DEM/CFD-DEM Modelling of Non-spherical Particulate Systems: Theoretical Developments and Applications. *Powder Technol.* **2016**, *302*, 108–152, doi:10.1016/j.powtec.2016.07.010.

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Paper B

Numerical Study of the 3D-Flow Characteristics during Compression Moulding of SMC

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NUMERICAL STUDY OF THE 3D-FLOW CHARACTERISTICS DURING COMPRESSION MOULDING OF SMC

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ABSTRACT

A numerical model for compression moulding of Sheet Moulding Compound is presented. The model is based on fluid mechanics and the SMC charge is modelled as a fluid with a viscosity that is dependent on the charge temperature, the fibre volume fraction of the material and the shear strain rate. Trends observed in the simulations regarding the shape of the flow front agree with experimental observations in previous studies. The simulations also yield that the type and magnitude of initial heating effects the initial flow to a large extent.

1 INTRODUCTION

The automotive industry faces, and will continue to face, significant challenges regarding emissions. In order to overcome these challenges, lighter vehicles are required. Composite materials presents one solution; however, the rapid cycle times often demanded by the automotive industry rule out many common methods. Compression moulding of Sheet Moulding Compound (SMC) is one process that is interesting in this context, given that it has advantages compared to many other methods both with regards to cycle times and costs. For use in the industry it is however required that both the process and the mechanical properties of the final part can be modelled accurately, due to the short development times and high demands on the properties of the part manufactured.

SMC comes in prefabricated sheets of resin and chopped fibres. These sheets are then cut into appropriate size and shape and placed inside the mould. As the mould is closed, the charge is melted and compressed to fill the mould and cure the resin. This is a rather complicated process to model for a number of reasons including: The intricate rheological properties of the charge, three-dimensional effects in the flow front, significant temperature gradients and the presence of chopped fibres that move and orientate as the charge flows. The details of the motions of the flow were studied by, among others, Odenberger et al [1] and Olsson et al [2].

The rheological properties of SMC has also been a topic for research and studied by e.g. Lee 1981 [3], Le Corre et al [4] and Dumont et al [5]. It is found that the main influence on the viscosity of the charge comes from the temperature, the strain rate and the fibre volume fraction. The empirical relations describing these were used by Kluge et al [6] in their work, in which the compression of SMC in a circular section was modelled, with the main focus being to correctly predict the pressure distribution. The flow was modelled fully three-dimensionally instead of being based on, for instance, Hele-Shaw formulations [7-8]. The work presented in this paper aims to expand this model into more complicated geometries, and also to include the air that is displaced during the moulding. This will also allow for more detailed studies of the temperature distribution and the flow field including flow front effects. A better understanding of the three-dimensional flow may lay ground for improved fibre orientation models being a major issue regarding the prediction of compression moulding of SMC.

Existing models for the fibre orientation are usually based on the work of Folgar and Tucker [9] and Advani and Tucker [10], which is in turn based on the concept of Jeffery orbits [11]. The general idea is that the fibres are modelled as single ellipsoidal particles, for which the equations of motion can be directly solved, with additional term added to account for the fibre-fibre interactions that are bound to occur when the volume fraction of fibres is high (> 20%). It is, however, well established that the model under-predicts the evolution of the fibre orientation [12-13] and several models have been suggested to rectify this, e.g. [13-14] but the results are still not satisfactory for a general case. Another issue that was discussed by Perez et al [15] is that Jeffery orbits are based on that the particles are able to rotate freely, which is not typically the case in SMC moulds. Thus, fibre orientation is not currently included in the model presented here and will be implemented in a later stage.

2 NUMERICAL MODELLING OF SMC

For the numerical simulations, the software ANSYS CFX 17 has been used. Two geometries are chosen for the study, representing two specific cases: the flow around a bend (Fig. 1) and the flow in and around a crossrib (Fig. 2), both of which are features that can be seen in real processing cases. In Fig. 1, the lower edge is an opening, and in Fig. 2, it is the edge furthest to the right. The other sidewalls use symmetry boundary conditions, while the upper and lower parts of the mould are solid walls with fixed temperatures.

The simulated geometries are divided into two parts, where one domain describes the initial placement of the SMC charge, and the other is filled with air and connected to an opening. When the

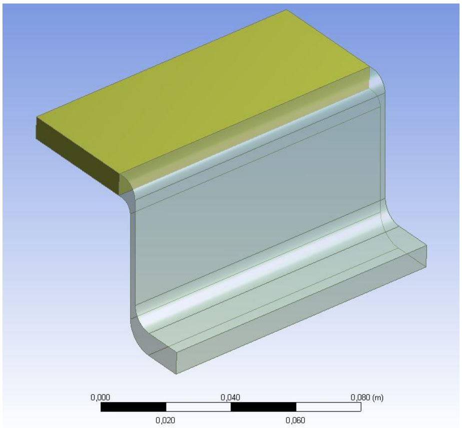


Figure 1: The bend. Highlighted area indicates where charge is located at start of simulation.

process starts, these domains are compressed in the height direction and the charge thus starts to move. The compression is then continued at a specified speed until the desired final thickness is reached. For all cases presented here, the speed is 2 mm/s.

For the temperature modelling, the initial temperature of the charge is 25 °C for the case with the ben and 80 °C for the crossrib (see Fig. 1 and 2), and the upper and lower parts of the mould have a temperature of 140 °C. The different temperatures of the two charges are used as a means of testing and demonstrating the effects of temperature on the flow. A preheating stage of 6 s is included, in which only the lower wall is heated, to account for the time required from layup until the pressing starts.

2.1 Equations

As was previously mentioned, the charge is modelled as a fluid with a viscosity that is dependent on the temperature, the shear rate and the fibre volume fraction of the SMC. One way to model this is according to:

$$\eta = 3\eta_0 \left(1 + 100 f_f + 1000 f_f^2\right) e^{-B\left(\frac{1}{T_0} - \frac{1}{T}\right)} \left(\frac{\dot{\varepsilon}}{\dot{\varepsilon}_0}\right)^{n-1} \left(1 + \dot{\gamma}^2\right)^{\frac{n-1}{2}} \quad (1)$$

, which is taken from Kluge [6]. Here η is the viscosity, f_f is the fibre volume fraction, *B* is a constant relating to the influence of temperature, *T* is the temperature, $\dot{\varepsilon}$ is the strain rate, $\dot{\gamma}$ is the shear strain rate, *n* is a power law constant and the subscript 0 denotes initial conditions.

2.2 Discretisation

The mesh consists entirely of hexahedral elements, since it was found that the quality of the mesh was best preserved through the compression. They are specified to have approximately 20 elements in the thickness direction.

3 RESULTS

The flow and temperature in the bend is first evaluated followed by investigations of the flow in the crossrib. Results are thereafter compared and discussed.

In the bend set-up preheating of the compound at the lower wall will induce a temperature gradient before the pressing is started, see Fig. 3 where the temperature distribution in the compound is presented consecutively during the preheating stage. When the pressing starts, see Fig. 3c, the temperature is thus higher in the lower part of the compound.

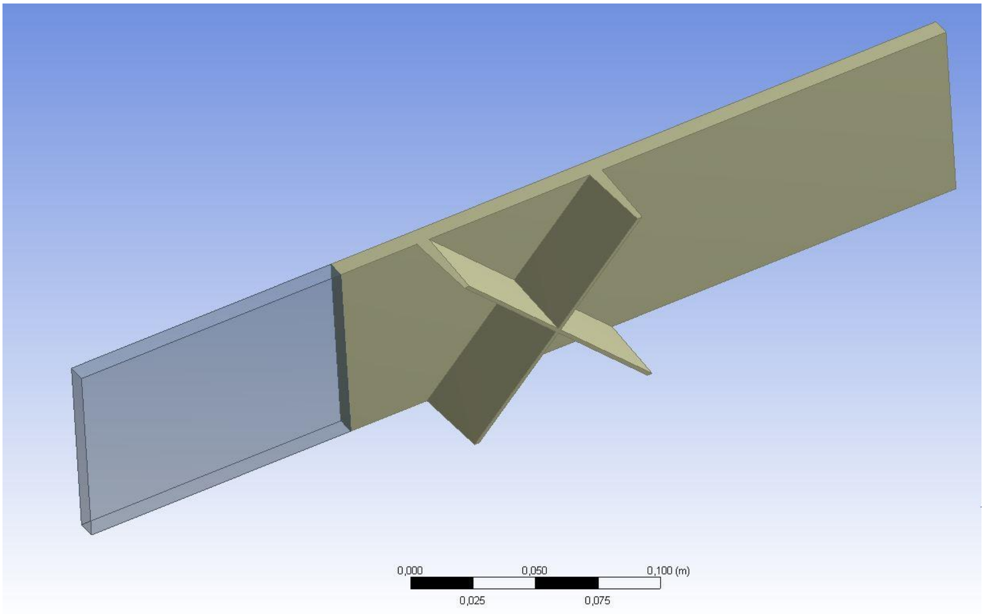
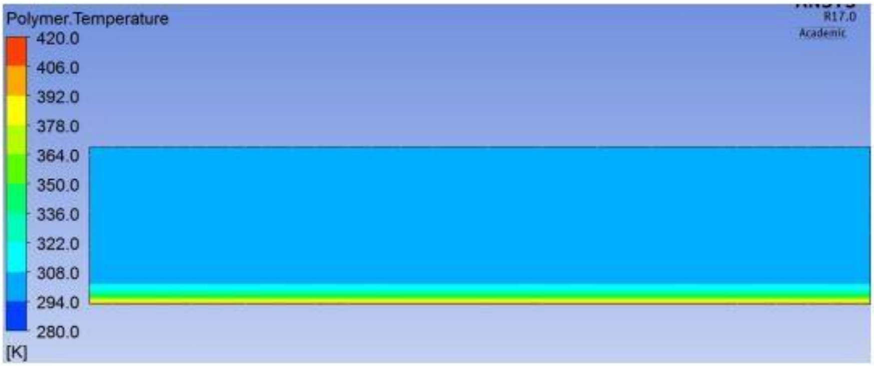
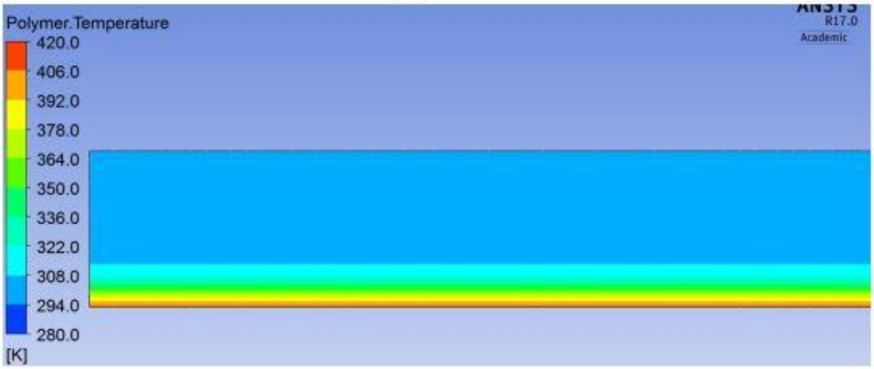


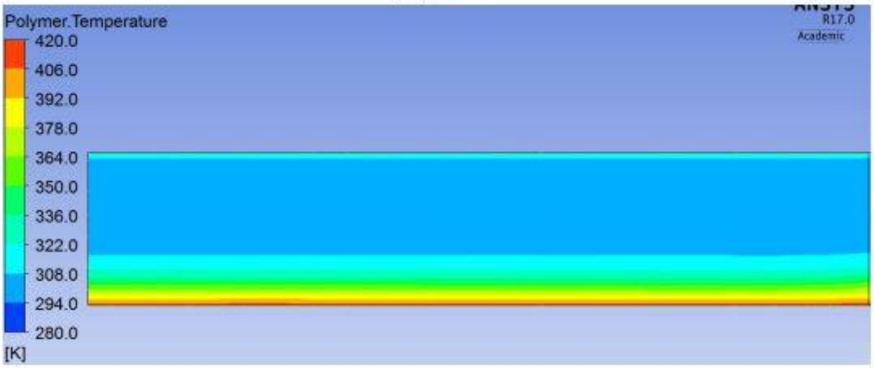
Figure 2: The crossrib. The transparent section indicates where the charge is initially placed.



(a) 1 s.



(b) 4 s.



(c) 6.1 s.

Figure 3: The temperature evolution during the heating phase. (a-b) before the pressing of the compound while (c) shows the temperature field just after the pressing has started.

Vector plots of the velocity field of the charge can be seen in Fig. 4, showing that initially most of the motion take place close to the lower wall, Figs 4a-d. This can be compared to the experimental al, results from Odenberger et al, where a similar effect was captured. It is worth noting, however, that in Odenberger this effect was seen more clearly at the upper wall as well. This difference can perhaps be attributed to differences between thermal conductivities and processing conditions. After the relatively dramatic initial flow the SMC moves smoothly over the corner but still an area in the outer corner is not filled, see Figs 4e-f.

To investigate this further the viscosity of the charge is also plotted, seen in Fig. 5a-f. A distinct area of lower viscosity originating from the heating of the compound can be observed at the flow front while the bulk of the charge still has a high viscosity (is not really melted) during the first 0.6 s of the compression.

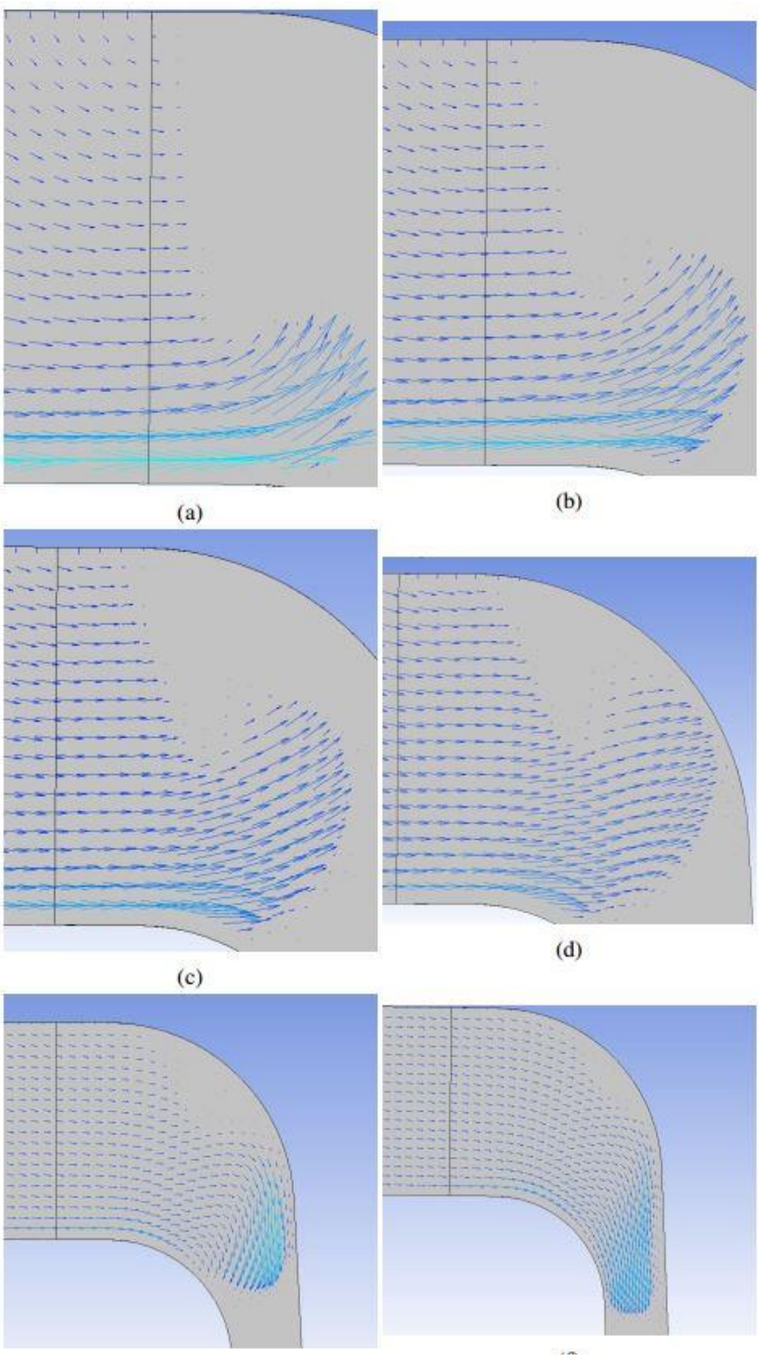


Figure 4: Vector plots of the evolution of the flow field around the corner. The time between each image is 0.1 s.

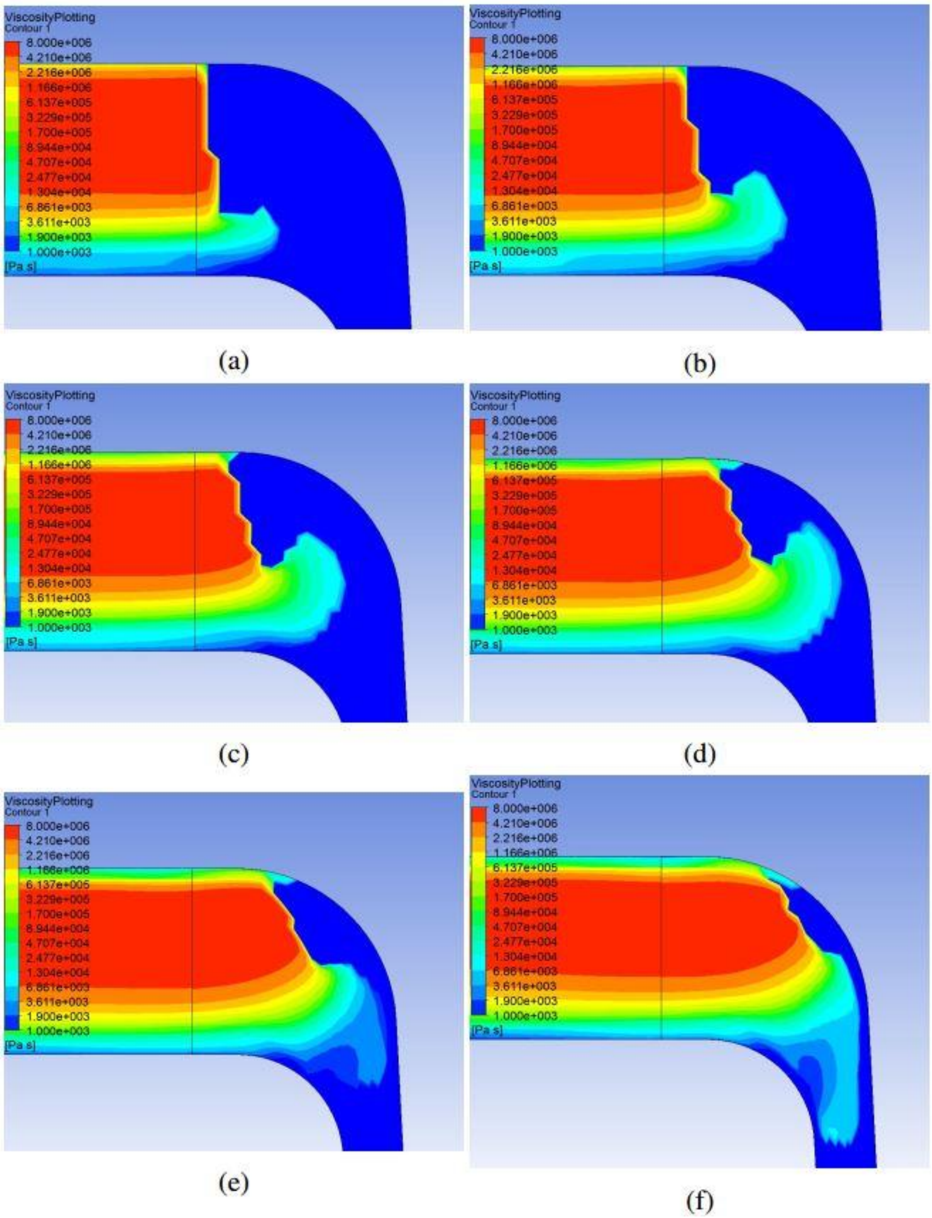


Figure 5: The evolution of the modelled viscosity of the charge. The step between each image is 0.1 s. Note the logarithmic scale.

Similar effects as seen for the bend (Fig. 4) can be seen in the crossrib in Fig. 6. The velocity vectors are mainly directed towards the upper wall initially, but the flow aligns towards the outlet later on. However, the layer closest to the wall does not leave as rapidly as in the previous example.

One possible reason for this is that the viscosity in the crossrib does not have as large gradients as for the bend geometry when the compression is initiated, compare Figs. 5 and 7. This is probably an effect of the fact that the compound temperature at the start of the preheating is 80 °C in the crossrib mould, while the initial charge temperature is only 25 °C in the mould with a bend. If Fig. 5 and 7 are compared, it can be seen that in the latter example the viscosity in the middle of the charge is significantly lower than in the example in Fig. 5. This suggests that for the case with the higher temperature charge, the temperature difference between the region near the wall and the middle region is not large enough to behave differently from a more normal squeeze flow.

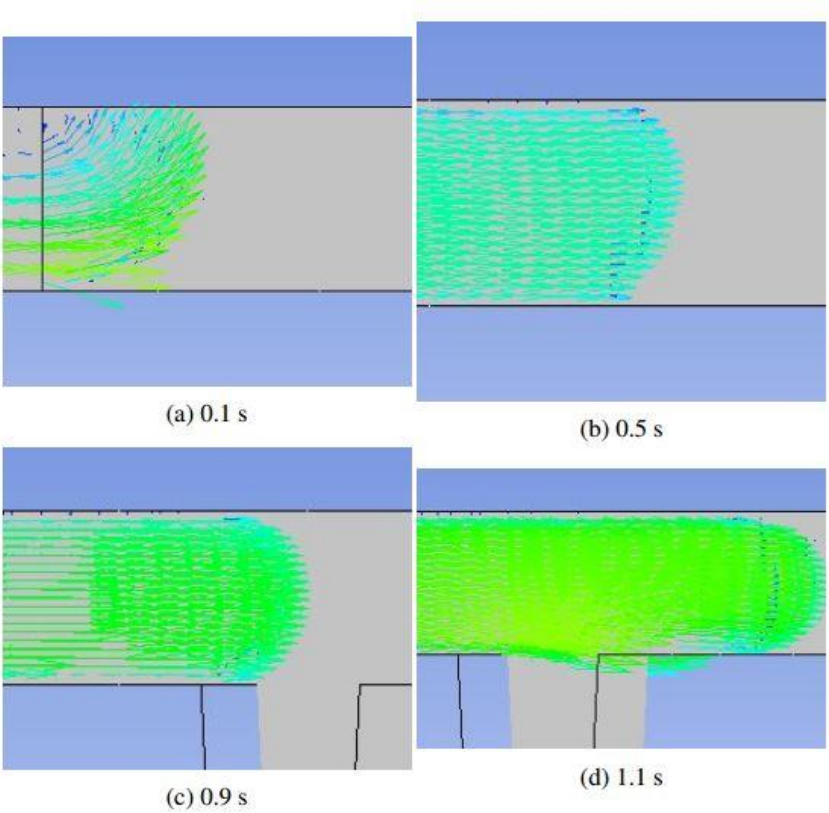


Figure 6: Vector plots of the velocity in the flow front. The times indicate the time that has passed since pressing started.

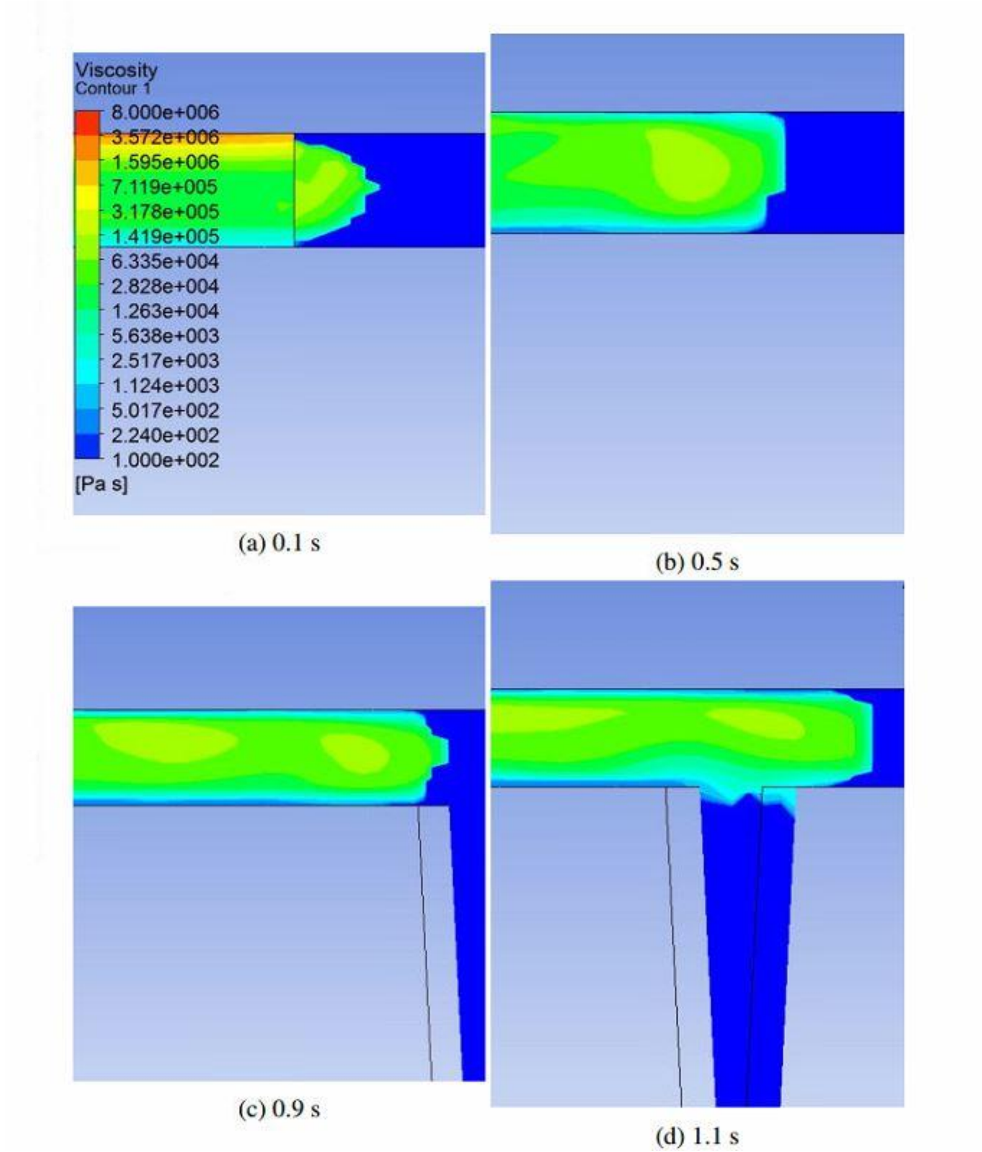


Figure 7: The modelled viscosity of the charge during pressing. The times indicate the time that has passed since pressing started. Note the logarithmic scale.

As previously discussed the bend geometry will, together with the compression, produce an observably laminar flow front with velocity vectors in the man flow direction after the bend. Velocity vectors in the flow direction are also seen in the crossrib mould, where the flow has almost obtained a laminar flow profile already before the ribs. Movement over the ribs does not seem to distinctly change the appearance of the flow front initially, as the fronts are similar before and after the rib.

9 CONCLUSIONS

A numerical model of compression moulding of SMC has been presented. The charge has been modelled as a fluid with a viscosity based on the temperature, the shear rate and the fibre volume fraction. Some results from the model have also been presented, and trends observed in the simulation results regarding the shape of the flow front agree with experimental observations in previous studies. The simulations also yield that the type and magnitude of initial heating effects the initial flow to a large extent.

The model is still in development, and there are several features that will be included in future works, such as a better interface between the air and the charge and some implementation for fibre orientation. Also the thermal boundary conditions need to be scrutinized.

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REFERENCES

[1] Odenberger, P. T., Andersson, H. M., & Lundström, T. S. (2004). Experimental flow-front visualisation in compression moulding of SMC. *Composites Part A: Applied Science and Manufacturing*, *35*(10), 1125–1134. https://doi.org/10.1016/j.compositesa.2004.03.019

[2] Olsson, N. E. J., Lundström, T. S., & Olofsson, K. (2009). Design of experiment study of compression moulding of SMC. *Plastics, Rubber and Composites*, *38*, 426–432.

[3] Lee, L. J., Marker, L. F., & Griffith, R. M. (1981). The rheology and mold flow of polyester sheet molding compound. *Polymer Composites*, *2*(4), 209–218. https://doi.org/10.1002/pc.750020412

[4] Le Corre, S., Orgéas, L., Favier, D., Tourabi, A., Maazouz, A., & Venet, C. (2002). Shear and compression behaviour of sheet moulding compounds. *Composites Science and Technology*, *62*(4), 571–577. https://doi.org/10.1016/S0266-3538(01)00151-8

[5] Dumont, P., Orgéas, L., Le Corre, S., & Favier, D. (2003). Anisotropic viscous behavior of sheet molding compounds (SMC) during compression molding, *19*, 625–646.

[6] Kluge, N. J., Lundström, T. S., Westerberg, L. g., & Olofsson, K. (2015). Compression moulding of sheet moulding compound: Modelling with computational fluid dynamics and validation. *Journal of Reinforced Plastics and Composites*, *34*(6), 479–492. https://doi.org/10.1177/0731684415573981

[7] Batchelor, G. K. (1967). *An Introdution to Fluid Mechanics*. Cambridge University Press.

[8] Lee, C., Folgar, F., & Tucker, C. L. (1984). Simulation of Compression Molding for Fiber-Reinforced Thermosetting Polymers. *Journal of Engineering for Industry*, *106*(2), 114. https://doi.org/10.1115/1.3185921

[9] Folgar, F., & Tucker, C. L. (1984). Orientation Behavior of Fibers in Concentrated Suspensions. *Journal of Reinforced Plastics and Composites*, *3*(2), 98–119. https://doi.org/10.1177/073168448400300201

[10] Advani, S. G., & Tucker, C. L. (1987). The Use of Tensors to Describe and Predict Fiber Orientation in Short Fiber Composites. *Journal of Rheology*, *31*(8), 751–784. https://doi.org/10.1122/1.549945

[11] Jeffery, G. B. (1922). The Motion of Ellipsoidal Particles Immersed in a Viscous Fluid. *Proceedings of the Royal Society A*, *102*, 161–179.

[12] Sepehr, M., Carreau, P. J., Moan, M., & Ausias, G. (2004). Rheological properties of short fiber model suspensions. *Journal of Rheology*, *48*(5), 1023–1048. https://doi.org/10.1122/1.1773783

[13] Wang, J., O'Gara, J. F., & Tucker, C. L. (2008). An objective model for slow orientation kinetics in concentrated fiber suspensions: Theory and rheological evidence. *Journal of Rheology*, *52*(5), 1179–1200. https://doi.org/10.1122/1.2946437

[14] Tseng, H.-C., Chang, R.-Y., & Hsu, C.-H. (2016). An objective tensor to predict anisotropic fiber orientation in concentrated suspensions. *Journal of Rheology*, *60*, 215–224.

[15] Perez, M., Scheuer, A., Abisset-Chavanne, E., Chinesta, F., & Keunings, R. (2016). A multi-scale description of orientation in simple shear flows of confined rod suspensions. *Journal of Non-Newtonian Fluid Mechanics*, *233*, 61–74. https://doi.org/10.1016/j.jnnfm.2016.01.011

Paper C

Fibre orientation for 3D-flow modelling of compression moulding of SMC

Manuscript

Fibre orientation for 3D-flow modelling of compression moulding of SMC

G. Alnersson, A-L Ljung, T. S, Lundström

October 27, 2021

Abstract

A numerical model for compression moulding of Sheet Moulding Compound is discussed. The model is a semi-empirical model based on rheological measurements on SMC that treats the fibres and the resin as a single medium. Flow results given by this model are then used as a basis for fibre orientation simulations that are then compared to experimental results. These results are well within the experimental margin of error.

1 Introduction

The transport sector faces, and will continue to face, significant challenges regarding emissions. In order to overcome these challenges, lighter vehicles than those produced today are required. Fibre reinforced polymer composites (FRPCs) presents one solution; however, the rapid cycle times often demanded by the automotive industry rule out many common methods used for these types of materials. Compression moulding of Sheet Moulding Compound (SMC) [1–3] is one process that is interesting in this context, given that it has advantages compared to many other methods both with regards to cycle times and costs. For use in the industry it is however required that both the process and the mechanical properties of the final part can be modelled accurately; this is a consequence of the short development times and high demands on the properties of the manufactured part. SMC comes in prefabricated sheets of resin and chopped fibres. These sheets are then cut into appropriate size and shape and placed inside the mould. As the mould is closed, the charge is melted and compressed to fill the mould and cure the resin. This is a rather complicated process to model for a number of reasons including: The intricate rheological properties of the charge, three-dimensional effects in the flow front, significant temperature gradients and the presence of chopped fibres that move and orientate as the charge flows. The details of the motions of the flow were studied by, among others, Odenberger et al [4] and Olsson et al [5] with the aim to minimize surface defects. 3D simulations of the filling stage during compression moulding of SMC were performed using commercial and all-purpose Computational Fluid Dynamic codes. With this approach pressure and temperature distributions can be predicted as well as weld lines. With focus on lightweight components stiffness and strength to weight ratios also come into play and consequently also both the spatial and orientation distributions of the chopped fibres.

Fibre orientation during compression moulding of SMC [6–16] is a very important aspect of the process, due to the influence on the mechanical properties of the finalized part. Such a multiphase flow with fibres may be studied with a one-way coupling, a two-way coupling or a four way coupling. One-way coupling implies that the motion of the fibres is affected by the flow, a two way coupling the fibres also influence the fluid flow (a relevant example is presented in [17]) and a four-way coupling implies that the motion of fibres is also, in addition to being affected by the flow, affected by other fibres. The one-way coupling is only valid for dilute suspensions which is not really the case for SMC. Still, this is the approach often taken when studying fibre orientation during compression moulding of SMC. The reason is that that modelling with two-way and four way coupling is challenging and time-consuming; instead the one-way coupling has been extended with extra terms to handle the particle-particle interactions. This is also the approach taken in this study.

In this paper the models used for fluid and fibre orientation will be described, and some results from a geometrically simple test case will be presented and discussed.

2 Methods

2.1 Fluid model

The flow is modelled fully three-dimensionally and is thus governed by the Navier-Stokes and continuity equations (see for instance [18]), which can be written as

$$\frac{Du_i}{Dt} = -\frac{1}{\rho}\frac{\partial p}{\partial x_i} + \frac{\eta}{\rho}\frac{\partial^2 u_i}{\partial u_i \partial u_j} \tag{1}$$

$$\frac{\partial u_i}{\partial x_i} = 0 \tag{2}$$

if it is assumed that the density of the material in constant (see for instance [19] for a discussion regarding this assumption). Here u_i denotes the velocity, $\frac{D}{Dt}$ is the material derivative, ρ is density, p is pressure and η is the viscosity.

The viscosity is described using the model suggested by Kluge et al [20], which was in turn based on the semi-empirical relations suggested by Le Corre et al [21] and Dumont et al [22], who experimentally studied the behaviour of the viscosity during the compression. Kluge suggested that the mixture of fibres and resin should be modelled as a single fluid with a temperature- and shear-dependent viscosity described as

$$\eta = 3\eta_0\left(1 + 100f_f + 1000f_f^2\right)e^{-B\left(\frac{1}{T_0}-\frac{1}{T}\right)}\left(\frac{\dot{\varepsilon}}{\dot{\varepsilon}_0}\right)^{n-1}\left(1+\dot{\gamma}^2\right)^{\frac{n-1}{2}}, \tag{3}$$

where η is the viscosity, f_f is the fibre volume fraction, B is a temperature constant, T is the temperature, $\dot{\varepsilon}$ is the strain rate, γ is the shear strain rate, n is a power law constant, and the subscript 0 indicates initial values.

Worth noting is that this model is strictly one-way, i.e. the orientation of the fibres does not influence the viscosity. Methods for this connection have been suggested [23]. As can be seen in Eq. (3) the viscosity is strongly temperature dependent; thusly the energy equation also needs to be solved

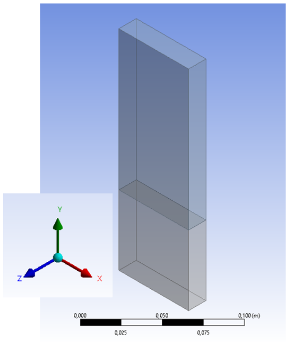


Figure 1: A schematic view of how the simulation domain for the fluid simulations is set up. Coordinate system has been enlarged for visibility.

$$\rho \frac{Dh}{Dt} = \frac{Dp}{Dt} + \tau_{ij} \frac{\partial u_i}{\partial x_j} + \frac{\partial}{\partial x_i} \left(\kappa \frac{\partial T}{\partial x_i} \right), \tag{4}$$

with h being the enthalpy, τ_{ij} is the viscous stress, κ is the thermal conductivity and T is the temperature.

This model has been implemented in the software ANSYS CFX 20.2, which uses the finite volume method (see for instance [24]). The structural setup used for the fluid simulations can be seen in Figure 1. The lower region indicates the initial position of the SMC charge, while the remainder of the domain is filled with air. In a normal press air would be able to escape through the sides of the mould; however, in this case this would result in all of the SMC material escaping through the sides, hence the sides of the mould are modelled as no-slip walls (i.e. the fluid has zero velocity relative to the wall) with the exception of the upper wall which is modelled as an opening so that the air can escape. All sidewalls as well as the upper and lower parts of the press are isothermal with a temperature of 140 degrees Celsius. When the pressing starts, the entire domain is compressed in the z direction with a specified velocity, which applies a force to the charge that results in displacement. When the numerical modelling of the flow is completed, a point cloud is generated in every time-step on the part of the domain containing the SMC charge. From these points files are generated that contain coordinates, velocity and velocity gradients for each of these points.

2.2 Fibre orientation

The method here used for calculation of fibre orientation is based on the work by Jeffery [25], who calculated the equations of motion for an ellipsoidal particle immersed in a fluid. This work was expanded by Folgar and Tucker [6] and Advani and Tucker [7], who added a rotary diffusion term that is intended to take particle-particle interactions into account without explicitly calculating them, according to

$$\frac{\mathrm{D}a_{ij}}{\mathrm{D}t} = -\frac{1}{2}\left(\omega_{ik}a_{kj} - a_{ik}\omega_{kj}\right) + \frac{1}{2}\lambda\left(\dot{\gamma}_{ik}a_{kj} + a_{ik}\dot{\gamma}_{kj} - 2\dot{\gamma}_{kl}a_{ijkl}\right) + 2D_r\left(\delta_{ij} - \alpha a_{ij}\right) \tag{5}$$

where a_{ij} is the orientation tensor, ω is the vorticity, $\dot{\gamma}$ is the shear strain rate and D_r is the rotary diffusivity. Worth noting is that Eq. (5) contains a fourth-order orientation tensor, which usually is handled using a closure approximation. Here the hybrid closure approximation suggested by Advani and Tucker [26] has been implemented

$$\bar{a}_4 \cong \bar{a}_{ijkl} = (1-f)\hat{a}_{ijkl} + f\tilde{a}_{ijkl}. \tag{6}$$

In Eq. (6), $\hat{a}_{ijkl}$ is the linear closure approximation (see also [27])

$$\hat{a}_{ijkl} = -\frac{1}{35}\left(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right) + \frac{1}{7}\left(a_{ij}\delta_{kl} + a_{ik}\delta_{jl} + a_{il}\delta_{jk} + a_{kl}\delta_{ij} + a_{jl}\delta_{ik} + a_{jk}\delta_{il}\right), \tag{7}$$

$\tilde{a}_ijkl$ is the quadratic closure approximation which is described as

$$\tilde{a}_ijkl = a_{ij}a_{jk}, \tag{8}$$

and f is a scalar measure of orientation that here is defined as

$$f = 1 - N\det\left(a_{ij}\right), \tag{9}$$

with N being equal to 27 for the three-dimensional cases discussed here. Using this method results in orientation tensors that describe the angles of the fibres.

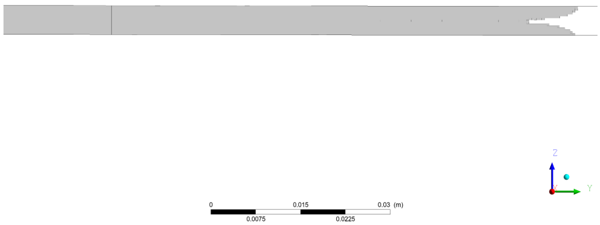
2.3 Experimental comparisons

The details of the results from the flow simulations, in particular the evolution of the flow front, will be qualitatively compared to the experimental results from Odenberger et al [4]. In these experiments SMC was moulded inside an open mould which allowed the tracing of the evolution of the flow front. It was observed that the outer layers of the SMC charge started flowing first creating an U-shaped flow front. It was assumed that this was a consequence of the temperature-dependent viscosity in conjunction with a quite steep temperature gradient in the thickness direction.

For a quantitative validation of the fibre orientation modelling, the experimental data from Advani and Tucker [8] is used. In their work flat plates were pressed using glass fibre SMC, and the pressing was done in such a way that the flow was close to unidirectional. The charges used for these pressings contained a fraction of lead glass fibres that were used as tracers. When these pressings are radiographed, the angles of the tracer fibres can be calculated and average values for the orientation tensors can be estimated. Several different cases were used with different degrees of filling of the base area of the mould: 33, 50, 66 and 100 percent were all tested.

(a) t=0.25 s

(b) t=0.5 s



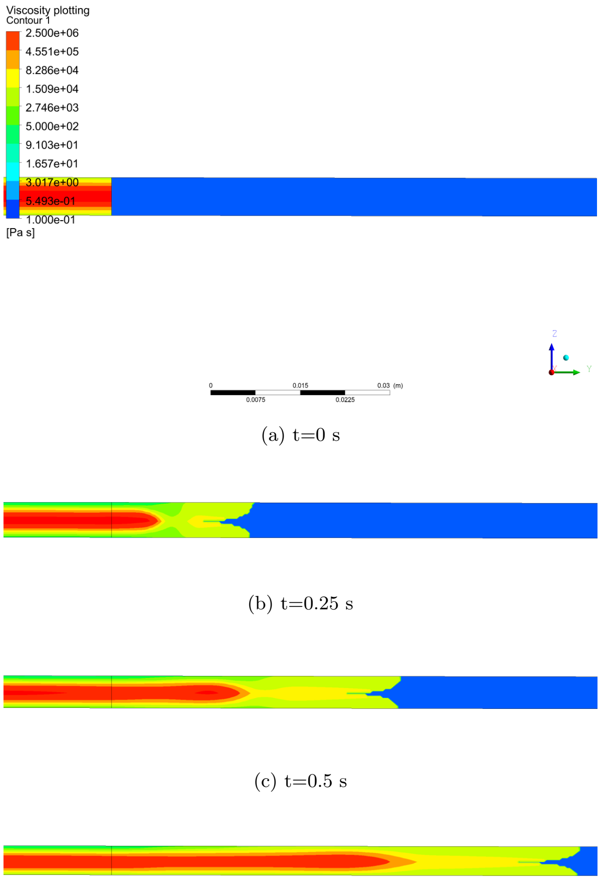
(c) t=0.75 s

Figure 2: Time evolution of the flow front of the SMC. The times indicated are time since pressing started.

3 Results and Discussion

Results from the evaluation of the flow can be seen in Figure 2. It can be observed that the flow starts in the regions closest to the upper and lower walls which creates an U-shaped flow front, in qualitative agreement with the experimental observations from Odenberger et al [4]. It is a reasonable conclusion that this is a consequence of the viscosity gradient, as can be seen in Figure 3, where the difference in viscosity at the time the pressing starts can be observed to be close to three orders of magnitude lower than that in the core of the flow.

The results from Advani and Tucker [8] can be seen alongside our numerical results for fibre orientation in Table 1. It is noted that while the simulated a_{12}-components are well within the experimental insecurities, the a_{11}-components, the components signifying alignment with the principal flow direction, are slightly lower than the experiments suggest. One possible explanation for this is that the experimental results, unlike our simulations, do not include the a_{33}-components, i.e. in the out-of-plane direction. Although not much movement is expected in the out-of-plane direction in this particular case, even relatively small variations could possibly influence the orientation tensors.



(a) t=0 s

(b) t=0.25 s

(c) t=0.5 s

(d) t=0.75 s

Figure 3: Time evolution of the viscosity of the SMC. The times indicated are time since pressing started.

Overall, however, the comparisons presented shows that the simulation procedure presented can give reliable results.

4 Conclusion

A 3D-flow model for the flows during compression moulding of SMC has been implemented. The model uses a semi-empirical description for the viscosity that

Table 1: Experimental results from Advani and Tucker [8] compared to numerical results of the average values in the domain of the noted components of the orientation tensors. The numbers given in the left column indicate the percentage of the surface area of the mould that is covered by material at the start of pressing.

	a_{11}	a_{12}
Experimental (50)	0.624 ± 0.13	0.024 ± 0.008
Simulated (50)	0.520 ± 0.03	0.030 ± 0.01
Experimental (67)	0.594 ± 0.09	0.013 ± 0.01
Simulated (67)	0.560 ± 0.03	0.010 ± 0.008

takes temperature, shear rate and fibre volume fraction into account. The results of the flow simulations are in good agreement with trends seen in experimental work. These flow results have been used as input for a 3D fibre orientation model, the results of which have been compared to experimental data from the literature. The fibre orientation results are well within the experimental margins of error.

References

[1] M. R. Barone and D. A. Caulk. Kinematics of Flow in Sheet Molding Compounds. *Polymer Composites*, 6, 1985.

[2] L. J. Lee, L. F. Marker, and R. M. Griffith. The rheology and mold flow of polyester sheet molding compound. *Polymer Composites*, 2(4):209–218, 1981.

[3] Johannes Görthofer, Nils Meyer, Tarkes Dora Pallicity, Ludwig Schöttl, Anna Trauth, Malte Schemmann, Martin Hohberg, Pascal Pinter, Peter Elsner, Frank Henning, Andrew Hrymak, Thomas Seelig, Kay Weidenmann, Luise Kärger, and Thomas Böhlke. Virtual process chain of sheet molding compound: Development, validation and perspectives. *Composites Part B: Engineering*, 169(December 2018):133–147, 2019.

[4] P. T. Odenberger, H. M. Andersson, and T. S. Lundström. Experimental flow-front visualisation in compression moulding of SMC. *Composites Part A: Applied Science and Manufacturing*, 35(10):1125–1134, 2004.

[5] N. E. J. Olsson, T. S. Lundström, and K. Olofsson. Design of experiment study of compression moulding of SMC. *Plastics, Rubber and Composites*, 38, 2009.

[6] F. Folgar and C. L. Tucker. Orientation Behavior of Fibers in Concentrated Suspensions. *Journal of Reinforced Plastics and Composites*, 3(2):98–119, 1984.

[7] S. G. Advani and C. L. Tucker. The Use of Tensors to Describe and Predict Fiber Orientation in Short Fiber Composites. *Journal of Rheology*, 31(8):751–784, 1987.

[8] S. G. Advani and C. L. Tucker. A numerical simulation of short fiber orientation in compression molding. *Polymer Composites*, 11(3):164–173, 1990.

[9] M. Kobayashi, K. Dan, T. Baba, and D. Urakami. Compression Molding 3D-Cae of Discontinuous Long Fiber Reinforced Polyamide 6 : Influence on Cavity Filling and Direct Fiber Simulations of Viscosity Fitting Methods. *20th International Conference on Composites Materials*, pages 1–12, 2015.

[10] J. H. Phelps and C. L. Tucker III. An anisotropic rotary diffusion model for fiber orientation in short- and long-fiber thermoplastics. *Journal of Non-Newtonian Fluid Mechanics*, 156:165–176, 2009.

[11] H.-C. Tseng, R.-Y. Chang, and C.-H. Hsu. Phenomenological improvements to predictive models of fiber orientation in concentrated suspensions. *Journal of Rheology*, 57(6):1597–1631, 2013.

[12] H.-C. Tseng, R.-Y. Chang, and C.-H. Hsu. An objective tensor to predict anisotropic fiber orientation in concentrated suspensions. *Journal of Rheology*, 60:215–224, 2016.

[13] Johannes Görthofer, Matti Schneider, Felix Ospald, Andrew Hrymak, and Thomas Böhlke. Computational homogenization of sheet molding compound composites based on high fidelity representative volume elements. *Computational Materials Science*, 174(October 2019):109456, 2020.

[14] N. Meyer, L. Schöttl, L. Bretz, A. N. Hrymak, and L. Kärger. Direct Bundle Simulation approach for the compression molding process of Sheet Molding Compound. *Composites Part A: Applied Science and Manufacturing*, 132(January):105809, 2020.

[15] Jan Teuwsen, Stephan K. Hohn, and Tim A. Osswald. Direct fiber simulation of a compression molded ribbed structure made of a sheet molding compound with randomly oriented carbon/epoxy prepreg strands—a comparison of predicted fiber orientations with computed tomography analyses. *Journal of Composites Science*, 4(4), 2020.

[16] M. Perez, D. Prono, C. Ghnatios, E. Abisset, J. L. Duval, and F. Chinesta. Advanced modeling and simulation of sheet moulding compound (SMC) processes. *International Journal of Material Forming*, 13(5):675–685, 2020.

[17] G. G. Lipscomb, M. M. Denn, D. U. Hur, and D. V. Boger. The flow of fiber suspensions in complex geometries. *Journal of Non-Newtonian Fluid Mechanics*, 26(3):297–325, 1988.

[18] Yunus A. Cengel and John M. Cimbala. *Fluid Mechanics: Fundamentals and Applications*. McGraw-Hill, third edition, 2014.

[19] D. Ferré Sentis, L. Orgéas, P. J.J. Dumont, S. Rolland du Roscoat, M. Sager, and P. Latil. 3D in situ observations of the compressibility and pore transport in Sheet Moulding Compounds during the early stages of compression moulding. *Composites Part A: Applied Science and Manufacturing*, 92:51–61, 2017.

[20] N. E. J. Kluge, T. S. Lundström, L. G. Westerberg, and K. Olofsson. Compression moulding of sheet moulding compound: Modelling with computational fluid dynamics and validation. *Journal of Reinforced Plastics and Composites*, 34(6):479–492, 2015.

[21] S. Le Corre, L. Orgéas, D. Favier, A. Tourabi, A. Maazouz, and C. Venet. Shear and compression behaviour of sheet moulding compounds. *Composites Science and Technology*, 62(4):571–577, 2002.

[22] P. J. J. Dumont, S. Le Corre, L. Orgéas, D. Favier, C. Gaborit, and P. Lory. Finite Element Implementation of a Two-Phase Model for Compression Molding of Composites. *Euro J Comput Mech*, 14(March):883–900, 2005.

[23] R. Bertóti and T. Böhlke. Flow-induced anisotropic viscosity in short FRPs. *Mechanics of Advanced Materials and Modern Processes*, 2017.

[24] Joel H. Ferziger, Milovan Peric, and Robert L. Street. *Computational Methods for Fluid Dynamics*. Springer, fourth edition, 2020.

[25] G. B. Jeffery. The Motion of Ellipsoidal Particles Immersed in a Viscous Fluid. *Proceedings of the Royal Society A*, pages 161–179, 1922.

[26] Suresh G. Advani and Charles L. Tucker. Closure approximations for three-dimensional structure tensors. *Journal of Rheology*, 34(3):367–386, 1990.

[27] George L. Hand. A theory of anisotropic fluids. *Journal of Fluid Mechanics*, 13(1):33–46, 1962.

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