Warpage modelling of carbon fibre-reinforced SMC components in automotive applications

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Abstract
This paper presents a finite element-based warpage simulation method for carbon fibre-reinforced SMC (C-SMC) components for automotive application. In the SMC process, one of the main problems is dimensional distortion of the composite component which is an inherent response of the residual stresses that occur due to chemical and thermal shrinkage of the thermoset resin. To tackle this problem, the curing and cooling behaviour of the composite needs to be predicted in a warpage analysis. For this purpose, material characterization is performed to obtain the thermal and chemical properties, and to parametrize the material models for cure kinetics and time- and temperature-dependent resin modulus. Additionally, material properties of the resin in the glassy and rubbery state, the mechanical properties of the fibres and the fibre volume content are required as input in the thermo-mechanical simulation of warpage in Abaqus. In conjunction with the mapped fibre orientation distributions from the SMC process simulation, local homogenization of the aforementioned properties is performed to correctly define the material behaviour during warpage. The warpage of complex automotive composite structure is analysed and a comparison between the experimentally measured and the numerically predicted displacement field is provided.

1. Introduction

Sheet Molding Compound (SMC) is a ready-to-mold, discontinuous fibre reinforced polymer made from thermoset sheets under pressure and temperature by compression molding. These SMC parts offer superior weight-specific properties at relatively low cost and the ability to form complex geometries during compression molding, which is not possible with continuous reinforcement. These properties make them attractive for applications in the aerospace and automotive industries. After manufacturing, process-induced deformations such as shrinkage or warpage can occur and lead to the loss of the component's dimensional stability. Therefore, it is important to perform numerical simulations of the different process steps, including SMC process simulation, mapping & homogenization, and warpage simulation, and to combine these steps to avoid loss of information. In this way, the process-induced deformations together with the accumulated residual stresses can be predicted in advance.

Due to the reorientation of the fibres as consequence of the compression molding process, it is necessary to take the fibre orientations into account in the warpage simulation. The simulation steps of process simulation, mapping and warpage simulation must therefore be linked together. This results in a consistent CAE chain which makes it possible to transfer the information between the simulation steps [1 - 4], as shown in Figure 1. Görthofer et al. [1] and Meyer et al. [2] already present CAE chains for SMC, but warpage of SMC was not yet included. As warpage simulation generally uses a different mesh than the process simulation, the use of an intermediate mapping step is required. The fibre orientation tensor field is imported from the process simulation [5, 6] and mapped onto the warpage mesh using the

Mapping library MpCCI MabLib [7]. All necessary interface operations, such as mapping, clustering of orientation states and homogenization, are bundled in a self-developed plugin for the commercial FE tool ABAQUS. The purpose of this manuscript is to present the FEM-based warpage methodology, including flow-induced process effects, and to demonstrate its application to a complex automotive component. The methodology is explained in Section 2, followed by numerical simulation and experimental validation in Section 3. For accurately predicting the warpage behaviour of C-SMC components, an anisotropic material model which is explained in Subsection 2.2 is implemented in Abaqus using UMAT subroutine.

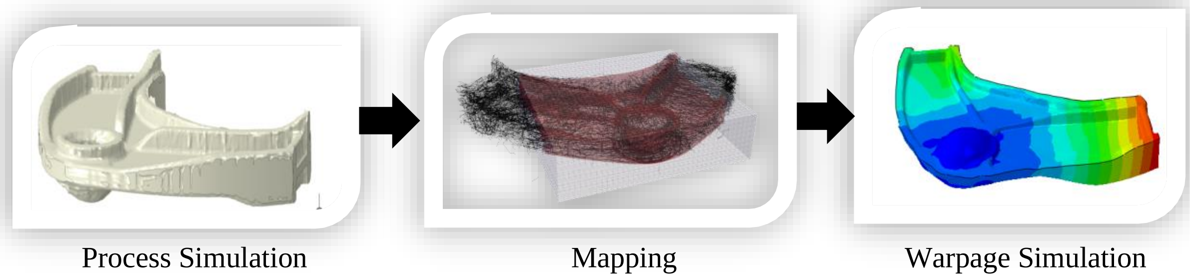

Figure 1. Virtual CAE chain using the example of an automotive control arm.

2. Methodology

2.1. Workflow

Warpage modelling for C-SMC requires the fibre orientation tensor distribution from moulding simulation which are mapped onto the warpage mesh [1, 4], cf. Fig. 2. The effective material properties of the composite are determined by homogenization of the mechanical, thermal and chemical properties in addition to the fibre orientation distributions from the process simulation [1, 2, 4], in order to correctly define the material behaviour during warpage. The material models and experimental characterization for cure kinetics, cure shrinkage, and cure- and temperature-dependent modulus are explained in Subsection 2.2.

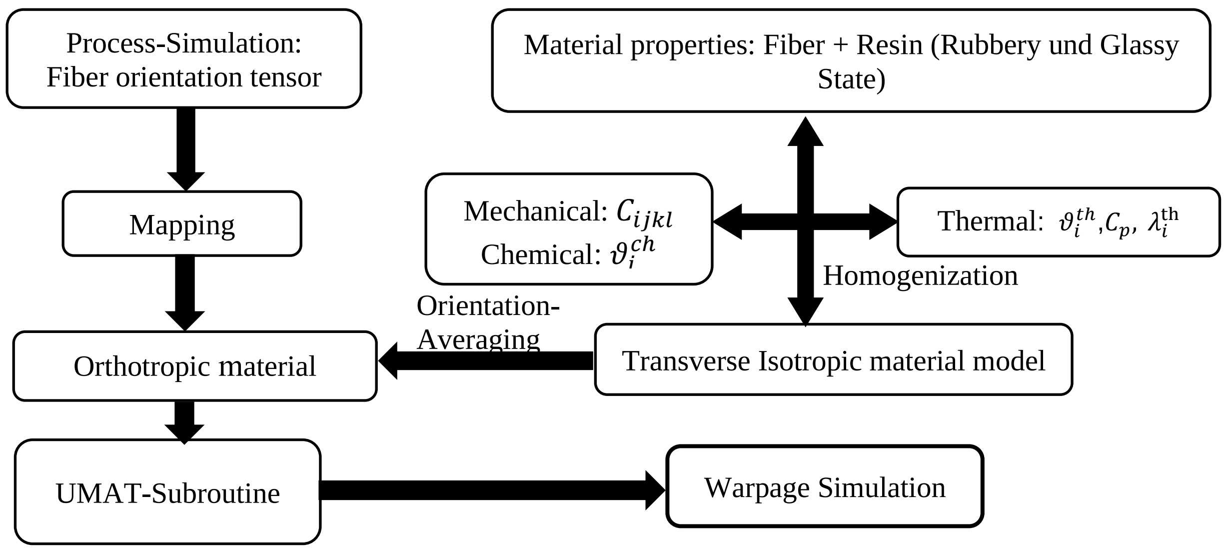

Figure 2. Workflow for the warpage modelling

In this work, the Tandon-Weng approach [8] is used for stiffness homogenization. It is based on the Eshelby tensor for unidirectional inclusions and considers the volume content of the fibres and the aspect ratio, as well as the stiffness of fibres and resin. This homogenization leads to the effective mechanical property of the stiffness tensor C_{ijkl}. For the thermal properties, the specific heat is averaged over the volume, as it is a scalar and isotropic property. The thermal conductivity is calculated using the Clayton approach [9]. For the coefficient of thermal expansion, Schapery's energy-based approach is used [10]. Chemical shrinkage is averaged over the volume. This homogenization leads to the effective thermal properties such as the thermal conductivity ϑ_i^{th} and the specific heat C_p, as well as the coefficient vector of the thermal expansion $\lambda_i^{\mathrm{th}}$and the chemical shrinkage ϑ_i^{ch}. The homogenized material properties are further averaged based on the fibre orientation tensor to describe the orthotropic behaviour required for SMC molded parts.

2.2. Material behaviour

The material system used for this analysis is a carbon fibre reinforced vinyl ester SMC stack with a weight percentage of 57% carbon fibres. This resin system was analysed with Toray using a differential scanning calorimeter for the cure kinetics and glass transition. A thermomechanical analysis was used for the coefficient of thermal expansion. A rheometer was used for the shrinkage measurement. Finally, a dynamic mechanical analysis was used for the elastic modulus characterization. The properties are summarized in the Table 1.

Table 1. Material Properties

	Fibre	Resin
Modulus (GPa)	250	Unrelaxed: 3.982 Relaxed: 1.125
Poisson’s Ratio	0.3	0.3
Density (kg/m^3)	1800	1162

2.2.1. Cure Kinetics

The curing kinetics are calculated using the Kamal-Malkin kinetics model [11], which calculates the rate of change by

$$\frac{d\alpha}{dt} = (K_1 + K_2 \cdot \alpha^m) \cdot (1-\alpha)^n \tag{1}$$

with the empirical parameters m and n [10]. The parameters K_1 and K_2 are often specified by an Arrhenius approximation in the form.

$$K_i = A_i \cdot \exp\left(-\frac{E_i}{R \cdot T}\right) \tag{2}$$

where α is the degree of cure, $\frac{d\alpha}{dt}$ is the cure rate, E_i is the activation energy, and A_i are fitting constants. The mechanical properties of the thermoset matrix material depend on the degree of cure, due to the crosslinking in the reaction kinetics of the matrix. The cure-dependence of the glass transition temperature T_g is modelled using the DiBenedetto approach [12,13],

$$\frac{T_{\mathrm{g}} - T_{\mathrm{g},0}}{T_{\mathrm{g},\infty} - T_{\mathrm{g},0}} = \frac{\lambda \cdot \alpha}{1-(1-\lambda)\cdot \alpha} \tag{3}$$

Here, λ is a model parameter which is 0.3. $T_{\mathrm{g},0}$= -44.04 °C and $T_{\mathrm{g},\infty}$=148.42 °C are the initial and final glass transition temperatures, respectively. $T_{\mathrm{g},0}$ is determined from cyclic DSC measurement, as shown in Figure 3. $T_{\mathrm{g},\infty}$ is the temperature at the maximum loss factor in the DMA measurement of temperature sweeps when the sample is fully cured, as shown in the Figure 4.

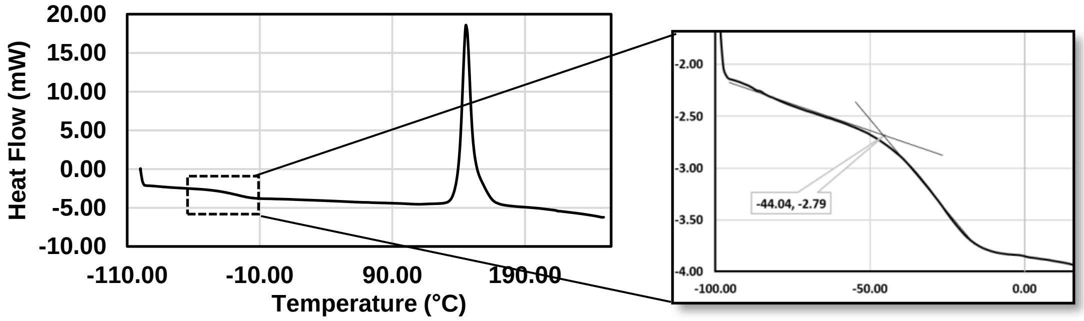

Figure 3. Cyclic DSC measurement

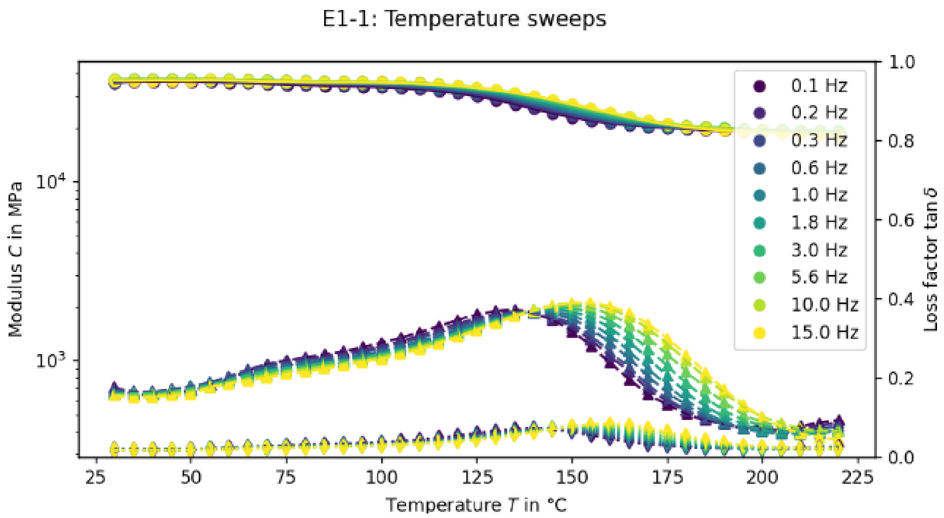

Figure 4. DMA Temperature Sweep

2.2.2. Thermal model

For the numerical simulation of the warpage of thermoset SMC components, thermal properties such as specific heat capacity, thermal conductivity, and coefficient of thermal expansion are required. These thermal properties are determined from material characterization in cooperation with Toray. The properties are given in Table 2.

Table 2. Thermal Properties

	Fibre	Resin
Coefficient of thermal expansion (1/K)	3.8×10^{-7}	3.908×10^{-5}
Specific Heat (J/Kg/K)	760	1310
Thermal Conductivity (m/W/K)	1.3	0.15

As discussed in subsection 2.2, the effective thermal conductivity is calculated with reference to Clayton [9]. For the coefficient of thermal expansion, the energy-based approach of Schapery [10] is used.

2.2.3. Chemical Shrinkage model

From PVT measurements, shrinkage is calculated to a value of -1.106% for the full cure cycle. The homogenization of chemical shrinkage is carried out using the volume averaging method, which is given by,

$$\vartheta_i^{\mathrm{ch}} = \varphi_{\mathrm{f}} \vartheta_{\mathrm{f},i}^{\mathrm{ch}} + \varphi_{\mathrm{m}} \vartheta_{\mathrm{m},i}^{\mathrm{ch}} \,. \tag{4}$$

Here $\vartheta_{\mathrm{f},i}^{\mathrm{ch}}$ and $\vartheta_{\mathrm{m},i}^{\mathrm{ch}}$ are the coefficients of chemical shrinkage for fibre and matrix, respectively. Since there is no shrinkage of the fibres, the effective shrinkage coefficient can be modified to

$$\vartheta_i^{\mathrm{ch}} = \varphi_{\mathrm{m}} \vartheta_{\mathrm{m},i}^{\mathrm{ch}} \tag{5}$$

with φ_{m}=1- φ_{f}. This is a simplified approach because the chemical shrinkage actually depends also on the fibre orientation.

2.2.4. Orthotropic CHILE Model

The Cure Hardening Instantaneously Linear Elastic (CHILE) model developed by Johnston is used to capture the stress evolution of the resin [14]. In case of C-SMC composite material, DMA experiments have shown a temperature dependency of the modulus. Therefore, the CHILE model is modified to fit a linear temperature dependency before the glass transition and used to model the cure-dependent mechanical behaviour of the composite material [14, 15, 16]. The models by Johnston [14] are extended and implemented to represent the orthotropic material behaviour for discontinuous carbon fibre reinforced vinyl ester resin SMC components. The stress evolution of the modified CHILE model is given by,

$$\sigma(t) = \int_0^t E(T,\alpha)\, \frac{\partial \varepsilon(\xi)}{\partial \xi}\, \mathrm{d}\xi, \tag{6}$$

where ξ is the time, $E(T,\alpha)$ is the instantaneous modulus of elasticity, which depends on the temperature T and the degree of cure $\alpha \in [0;1]$. The modified CHILE model assumes a monotonic increase in the resin modulus during curing according to

$$E(T,\alpha) = \begin{cases} E_1, & T^* < \Delta T_{\mathrm{c}_1} \\ E_2 + \dfrac{T^* - \Delta T_{\mathrm{c}_2}}{\Delta T_{\mathrm{c}_1} - \Delta T_{\mathrm{c}_2}} \,(E_1 - E_2), & \Delta T_{c_1} \le T^* < \Delta T_{\mathrm{c}_2} \\ E_3 + \dfrac{T^* - \Delta T_{\mathrm{c}_3}}{\Delta T_{\mathrm{c}_2} - \Delta T_{\mathrm{c}_3}} \,(E_2 - E_3), & \Delta T_{c_2} \le T^* < \Delta T_{\mathrm{c}_3} \\ E_3, & T^* \ge \Delta T_{\mathrm{c}_3} \end{cases}, \tag{7}$$

with $T^* = T - T_g$. The glass transition temperature T_g is calculated according to Equation (3). In DMA measurements, temperature sweep is carried out on carbon fibre reinforced SMC composite sample from 20 °C to 220 °C at frequency 1 Hz. Figure 5 reveals a tri-linear temperature dependency of the modulus of fibre reinforced vinyl ester resin. The modified CHILE model is fitted to the DMA experiments yielding the parameters: $\Delta T_{\mathrm{c}_1} = -116.82\ \text{°C}$, $\Delta T_{\mathrm{c}_2} = -18.37\ \text{°C}$, $\Delta T_{\mathrm{c}_3} = 22.75\ \text{°C}$, $E_1 = 34189.2\ \text{MPa}$, $E_2 = 30906.99\ \text{MPa}$, $E_3 = 16637.2\ \text{MPa}$. In this model, the rubbery modulus E_3 is active as long as T_{g} has not exceeded the current temperature by a certain value ΔT_{c_3}. The stiffness is equal to the glassy modulus E_1 if the temperature T reaches a value below T_{g} - ΔT_{c_1} during cooling.

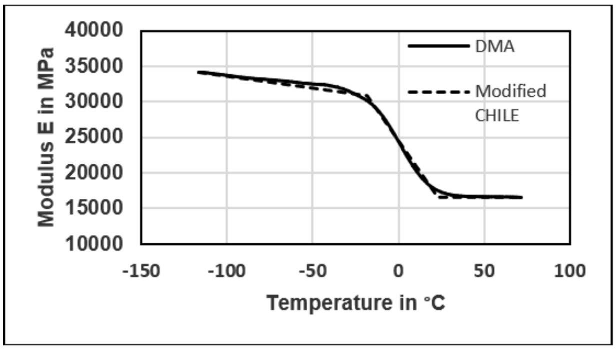

Figure 5. Temperature dependence of Modulus fitted to DMA.

2.2.5. Total strain

In the SMC process, the component undergoes chemical and thermal shrinkage in addition to the mechanical deformations, e.g. caused by the holding pressure. Thus, the complete change in elongation is given by,

$$\Delta\varepsilon_{ij} = \Delta\varepsilon_{ij}{}^{\text{mech}} + \Delta\varepsilon_{ij}{}^{\text{th}} + \Delta\varepsilon_{ij}{}^{\text{ch}} . \tag{8}$$

The change in thermal expansion is given by,

$$\Delta\varepsilon_{ij}{}^{\text{th}} = \vartheta_i^{\text{th}} \Delta T . \tag{9}$$

The change in chemical elongation is given by,

$$\Delta\varepsilon_{ij}{}^{\text{ch}} = \vartheta_i^{\text{ch}} \Delta\alpha . \tag{10}$$

A subroutine was created for the modified CHILE model and implemented in ABAQUS. The homogenization is performed according to the method presented by Görthofer et al [1, 2] as explained in the Subsection 2.1.

2.2.6. Reverse Homogenization

The characterization is done on the C-SMC composite material. Therefore, a reverse homogenization is carried out to get the neat resin properties [18]. This is an iterative process in which the properties of the carbon fibre and the C-SMC composite material are known, and the resin properties are calculated. The workflow for the reverse homogenization is shown in Figure 6.

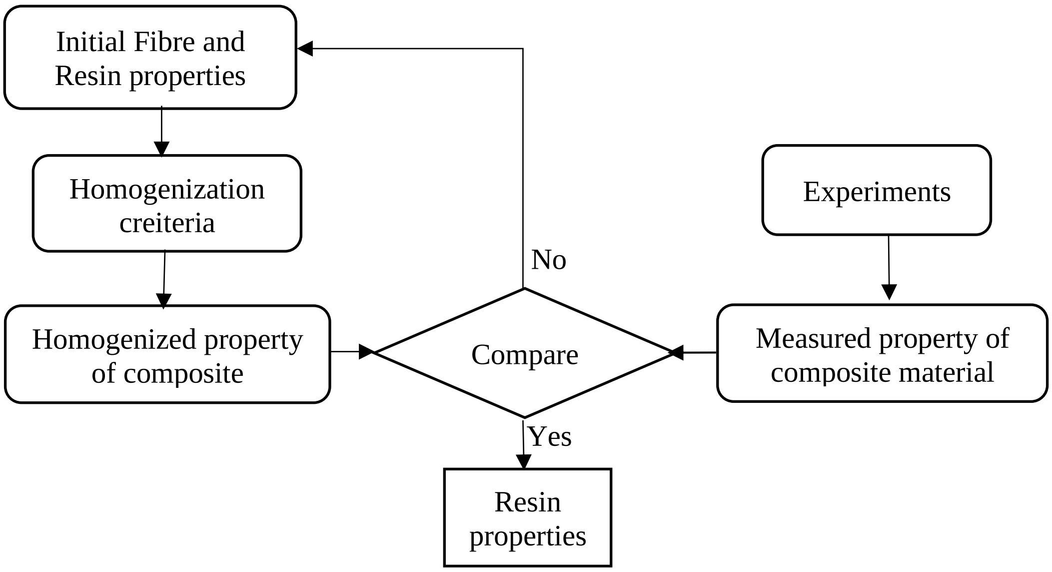

Figure 6. Reverse homogenization method

3. Numerical Simulation and Experimental Validation

The warpage analysis begins immediately after mold filling and includes the process steps of mold holding, curing, transfer and cooling outside the mold. The warpage analysis is carried out with the FE software ABAQUS 2021 (Dassault Systémes, USA). The simulation model is a section of a control arm of an automotive component, as shown in Figure 7. There are four steps in the simulations, namely mold holding, curing, transfer and cooling. During the mold holding and curing step, the displacements are blocked on the entire surface of the component, as it is still in the closed mold during the actual process. The surface temperature is set at a constant 140 °C. The curing step lasts 360 seconds, followed by a transfer step for 5 seconds and then a cooling step outside the mold. During cooling, a convection boundary condition is specified for the temperature field. The effective material properties are determined using the described schemes. For the mechanical model, the modified CHILE model is used in an orthotropic formulation. The orientation distribution is clustered into 100 sub-regions based on the fibre orientation tensors from mould filling simulation. According to the 100 material sections, 100 orthotropic materials are created that describe the thermomechanical material behaviour for the corresponding fibre orientation state.

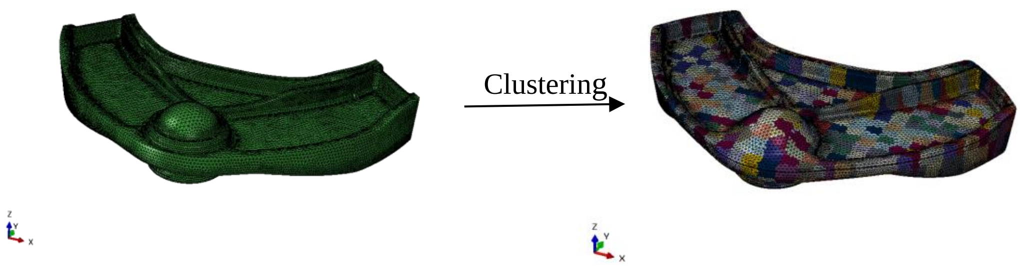

Figure 7. FE model of SMC Automotive suspension control arm showing orthotropic material clustering

An SMC suspension control arm was manufactured at Fraunhofer ICT, and measurements are conducted using GOM 3D ATOS scanner. Figure 8 shows a comparison between experimentally measured and numerically predicted displacements of the suspension control arm. The left-side figure shows the deviation of the manufactured part over the nominal geometry, and the right-side figure shows the deviation of the predicted shape of the component over the nominal geometry. The different deviation points in the figure indicate displacement values at specific locations. By comparison, it can be seen that the displacement values are qualitatively in reasonable agreement with the experimental results, but simulation underpredicts the deformation. In future work, the packing step after complete mold filling will be considered, which takes into account the additional holding pressure and may thus reduce the difference between simulation and experiment.

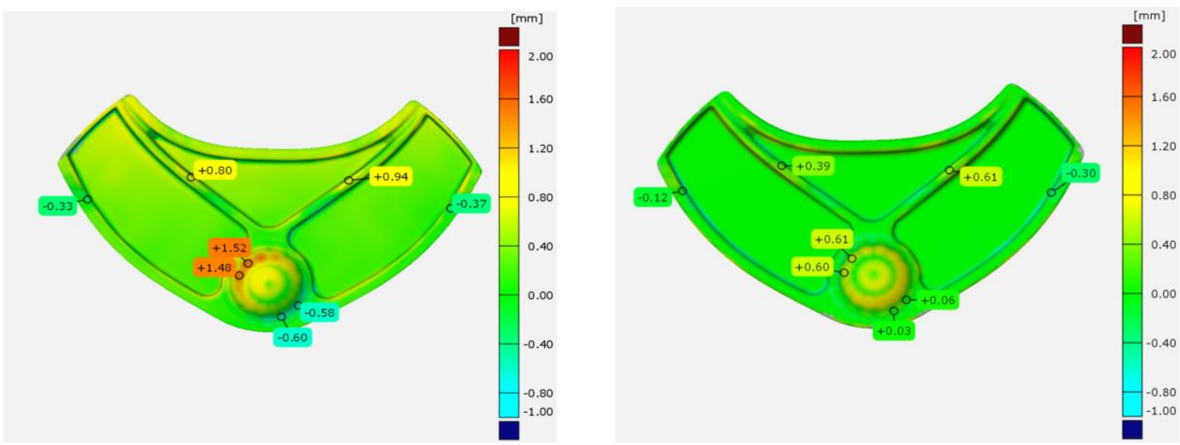

Figure 8. Comparison of experimentally measured (left) and numerically predicted (right) process-induced displacements of the SMC suspension control arm.

4. Conclusion

An orthotropic modified CHILE model has been implemented for process-induced warpage simulation of SMC components. The model is able to capture the distortion of fibre-reinforced SMC component as a function of process parameters, process-induced fibre orientation distributions and curing reaction. A consistent CAE chain approach is used to transfer the moulding simulation results onto the warpage mesh via mapping. The simulation methodology is applied for stress-deformation analysis of an automotive component suspension control arm, produced by compression molding of discontinuous carbon fibre-reinforced vinyl ester thermoset. The resulting fibre orientation distribution affects the warpage simulation results such as residual stresses and final shape of the part. The experimental results are qualitatively in good agreement with the deformations predicted by the simulations. However, the simulation underpredicts the deviation. In the future, a further developed viscoelastic material model for the matrix can also be used to capture the time-dependent behaviour of the matrix more accurately.

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References

[1] Görthofer, J., Meyer, N., Pallicity, T.D., Schöttl, L., Trauth, A., Schemmann, M., Hohberg, M., Pinter, P., Elsner, P., Henning, F. and Hrymak, A., 2019. Virtual process chain of sheet molding compound: Development, validation and perspectives. *Composites Part B: Engineering*, *169*, pp.133-147.

[2] Meyer N, Gajek S, Görthofer J, Hrymak A, Kärger L, Henning F, Schneider M, Böhlke T, 2023: A probabilistic virtual process chain to quantify process-induced uncertainties in Sheet Molding Compounds. *Composites Part B: Engineering, 249*, p. 110380.

[3] Kärger, L., Bernath, A., Fritz, F., Galkin, S., Magagnato, D., Oeckerath, A., Schön, A. and Henning, F., 2015. Development and validation of a CAE chain for unidirectional fibre reinforced composite components. *Composite Structures*, *132*, pp.350-358.

[4] Gorde, S.S., Krauß, C., Bartkowiak, M. and Kärger, L., 2022. CAE-Simulationskette zur Werkzeug- und Prozessauslegung von Carbonfaser-SMC-Bauteilen. In *NAFEMS DACH Regionalkonferenz 2022: Konferenz für Berechnung & Simulation im Engineering, 4.-6. Oktober 2022, Bamberg, D* (p. 142).

[5] Meyer N, Ilinzeer S, Hrymak AN, Henning F, Kärger L: Non-isothermal direct bundle simulation of SMC compression molding with a non-Newtonian compressible matrix. Journal of Non-Newtonian Fluid Mechanics 310: 104940, 2022.

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

[7] Wolf, K., Bayrasy, P., Brodbeck, C., Kalmykov, I., Oeckerath, A. and Wirth, N., 2017. MpCCI: Neutral interfaces for multiphysics simulations. In *Scientific Computing and Algorithms in Industrial Simulations* (pp. 135-151). Springer, Cham.

[8] Tandon, G.P. and Weng, G.J., 1984. The effect of aspect ratio of inclusions on the elastic properties of unidirectionally aligned composites. *Polymer composites*, *5*(4), pp.327-333.

[9] Clayton, W., 1971. Constituent and composite thermal conductivities of phenolic-carbon and phenolic-graphite ablators. In *12th Structures, Structural Dynamics and Materials Conference* (p. 380).

[10] Schapery, R.A., 1968. Thermal expansion coefficients of composite materials based on energy principles. *Journal of Composite materials*, *2*(3), pp.380-404.

[11] Kamal, M.R. and Sourour, S., 1973. Kinetics and thermal characterization of thermoset cure. *Polymer Engineering & Science*, *13*(1), pp.59-64.

[12] DiBenedetto, A.T., 1987. Prediction of the glass transition temperature of polymers: a model based on the principle of corresponding states. *Journal of Polymer Science Part B: Polymer Physics*, *25*(9), pp.1949-1969.

[13] Pascault, J.P. and Williams, R.J.J., 1990. Glass transition temperature versus conversion relationships for thermosetting polymers. *Journal of Polymer Science Part B: Polymer Physics*, *28*(1), pp.85-95.

[14] Johnston, A.A., 1997. *An integrated model of the development of process-induced deformation in autoclave processing of composite structures* (Doctoral dissertation, University of British Columbia).

[15] Johnston, A., Vaziri, R., & Poursartip, A. (2001). A plane strain model for process-induced deformation of laminated composite structures. *Journal of composite materials*, *35*(16), 1435-1469

[16] Khoun, K., 2009. Process-induced stresses and deformations in woven composites manufactured by resin transfer moulding.

[17] Advani, S.G. and Tucker III, C.L., 1987. The use of tensors to describe and predict fiber orientation in short fiber composites. *Journal of rheology*, *31*(8), pp.751-784.

[18] Gandhi, U., Song, Y.Y. and Mandapati, R., 2017. Semiempirical approach to predict shrinkage and warpage of fiber-reinforced polymers using measured material properties in finite element model. *Journal of Thermoplastic Composite Materials*, *30*(9), pp.1303-1319.