FIBER BREAKAGE MODELING BASED ON HYDRODYNAMIC FORCES IN MACROSCOPIC PROCESS SIMULATIONS

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Abstract: *Injection molding is one of the most important processes for manufacturing parts from discontinuous fiber reinforced polymers. Fiber length and orientation do not only influence the final structural behavior in an anisotropic way, but also the flow field and hence the mold filling process. Therefore, fiber length distribution and fiber breakage modeling are important aspects of an adequate process simulation. For fiber breakage modeling, hydrodynamic forces from matrix on fibers are considered within this work. Knowing the flow field and fiber orientation distributions of the homogenized material, flow-induced hydrodynamic forces on the fibers can be calculated. The fiber orientation tensor is used to determine reference fibers in every element. Based on this information an advanced approach for fiber breakage modelling is proposed. The fiber length distribution in the final part is compared to experimental data of a reactive injection molding process, showing good agreement.*

Keywords: Discontinuous fiber reinforced polymers; injection molding simulation; hydrodynamic forces; fiber breakage

1. Introduction

Injection molding of fiber reinforced polymers is one of the most important processes for manufacturing discontinuous reinforced polymer parts. Due to the option of full automatization in combination with realizing complex geometries, it is widely used in industry and was in the focus of several scientific publications in the last decades [1]. The process is transient and non-isothermal, and the materials show a complex chemo-thermal viscosity behavior, which is in case of fiber reinforcement also anisotropic. To ensure and optimize the manufacturing process, simulation is an important tool. An adequate process simulation has to focus on the non-Newtonian and chemo-thermal matrix material behavior, but also on the fibers [2]. Fiber orientation influences the mechanical behavior during mold filling and in the final part. This also applies to the fiber length, having crucial impact on viscosity and impact strength.

Fibers may break during processing. In literature, buckling is named as dominant phenomena for fiber breakage, although there are other effects [3, 4]. The shortening of fibers influences the viscosity behavior of the material and hence the flow field, which vice versa influences the forces acting on the fibers and therefore fiber breakage. Consequently, an adequate process simulation must include both anisotropic, fiber dependent flow modeling and fiber breakage modeling [5].

Since the numerical effort for performing a process simulation with individual fibers on part level is too high, the fiber orientation distribution is represented by an orientation tensor in most cases [6]. Unfortunately, no information on individual orientation and position of fibers is known by applying this tensorial approach. Hence, forces depending on position, orientation and contact of fibers, must be approximated. Our previous work [5, 7] presents approaches to calculate hydrodynamic and fiber-contact forces in macroscopic simulations with orientation tensors, by using eigenvectors of the orientation tensor as reference fibers. These forces are used in the present work to approximate the occurrence of fiber breakage.

Today's fiber breakage simulation approaches focus on buckling as phenomenon for fiber breakage. One of the most applied models in macroscopic simulations is the one presented by Phelps et al. [8]. Here, the acting forces are based on the work of Dinh and Amstrong [9], representing forces with slender body analysis. Based on this, a buckling index is determined and an empirical function describes the amount of buckling fibers, which break within a control volume. Within this work, a novel approach for fiber breakage simulation in macroscopic process simulations is presented. The approach is based on the work of Phelps et al., but with a different approach for force calculation and with the use of eigenvectors as reference fibers.

2. Theory

The fiber breakage modeling is based on reference fibers, which are represented by the eigenvectors ϑ_i of the second order orientation tensor. Hydrodynamic forces acting from the flow field on the fibers are approximated with the eigenvectors and are used for force calculation in the fiber breakage model. The hydrodynamic force F_i^{hyd} is split into a drag part, due to the relative velocity between fibers and polymer and a lift part, since the fibers are non-spherical. Based on Stokes law, the drag force F_i^{d} is approximated by

$$F_i^{\mathrm{d}} = 3\pi\eta_{\mathrm{M}} d_{\mathrm{f}} k_{\mathrm{d}} \Delta U_i, \tag{1}$$

with η_{M} being the matrix viscosity, d_{f} the fibers diameter, k_{d} a geometry-dependent fitting factor and ΔU_i the relative velocity. The fitting factor is given by

$$k_{\mathrm{d}} = 1 - \alpha(r_{\mathrm{f}} - 1)\cos(2\phi) + \beta(r_{\mathrm{f}} - 1), \tag{2}$$

with $\alpha = 0.09$, $\beta = 0.3125$, r_{f} being the aspect ratio of the fibers and ϕ the angle between ϑ_i and ΔU_i. A derivation for Eq. (1) and (2) is given by Meyer et al. [10, 11]. The definition of the relative velocity ΔU_i is given in our previous work [5, 7].

Similar to the drag force, the lift force F_i^{li} is approximated by

$$F_i^{\mathrm{li}} = 3\pi\eta_{\mathrm{M}} d_{\mathrm{f}} k_{\mathrm{li}} \|\Delta U_i\| [\![p_i]\!], \tag{3}$$

with

$$k_{\mathrm{li}} = \alpha(r_{\mathrm{f}} - 1)\sin(2\phi) \tag{4}$$

and

$$p_i = (\vartheta_i \times [\![\Delta U_i]\!]) \times [\![\Delta U_i]\!]. \tag{5}$$

The operator $[\![\cdot]\!]$ indicates that the vectors are normed. The derivation of the lift force is also given by Meyer et al. [10, 11]. In summary it is

$$F_i^{\mathrm{hyd}} = F_i^{\mathrm{d}} + F_i^{\mathrm{li}} = 3\pi\eta_{\mathrm{M}} d_{\mathrm{f}} (k_{\mathrm{d}} \Delta U_i + k_{\mathrm{li}} \|\Delta U_i\| [\![p_i]\!]). \tag{6}$$

This eigenvector-based approach for calculating hydrodynamic forces in the homogenized material is verified with numerical experiments in our previous work [7].

The assumptions for fiber breakage are:

- Fibers break due to buckling.
- Fibers break only in one point, so one fiber breaks only in two parts.
- Until buckling, fibers are perfect, rigid cylinders.
- There is a defined minimum fiber length, which cannot be undercut.
- There is a defined number of possible fiber lengths.
- Fiber-fiber contact forces are neglected.

The fiber forces, induced by the hydrodynamic load may lead to fiber buckling, and an amount of the fibers which buckle will also break. The forces are calculated on reference fibers, represented by the eigenvectors, therefore the fiber breakage modeling is also applied on the eigenvectors. In a first step it is determined if the fibers are under compression or tension, so if they may buckle or not, by checking if they are in the so-called Jeffery orbit, defined as

$$D_{ij}\vartheta_i\vartheta_j < 0, \tag{7}$$

with D_{ij} being the strain rate tensor. This is performed three times, once for each eigenvector. Afterwards it is determined if the forces are large enough to enable buckling in the fibers by

$$B = \frac{\hat{F}^{\mathrm{hyd}}}{F^{\mathrm{bu}}} \geq 1, \tag{8}$$

where $\hat{F}^{\mathrm{hyd}} = \vartheta_i F_i^{\mathrm{hyd}}$ since only the force component in fiber direction is relevant for buckling. The critical force for buckling is defined as

$$F^{\mathrm{bu}} = \pi^3 E_{\mathrm{f}} d_{\mathrm{f}}^4 / \left(64 L_{\mathrm{f}}^2\right), \tag{9}$$

with fiber Youngs modulus E_{f} and fiber length L_{f}. F^{bu} is determined independently for each fiber length. The buckling index B is calculated three times for each fiber length, once for every eigenvector. The ongoing calculations for fiber breakage modeling are adapted from the procedure presented by Phelps et al. [8]. Based on the buckling index, a breaking probability P_k is defined as

$$P_k = \begin{cases} 0, & B_k < 1 \quad \text{or} \quad D_{ij}\vartheta_{ik}\vartheta_{jk} \geq 0 \\ C\dot{\gamma}\left(1 - \exp(1 - B_k)\right), & B_k \geq 1 \quad \text{and} \quad D_{ij}\vartheta_{ik}\vartheta_{jk} < 0' \end{cases} \tag{10}$$

with the breakage coefficient C and the scalar shear rate $\dot{\gamma}$. The index $k \in \{1,2,3\}$ indicates the different eigenvectors ϑ_{ik}. To sum up the breakage probability within one cell, the eigenvector-specific probabilities are weighted with the corresponding eigenvalues,

$$P = \lambda_k P_k. \tag{11}$$

Whenever fibers break, new and shorter fibers are created. This ‘child generation’ must be considered in a constitutive modeling approach. It is assumed that fibers break only into two smaller parts within this work. Phelps et al. [8] define the child generation rate R_{nm} as probability density function (PDF), representing the position of the breaking point, so

$$R_{nm} = \varrho_m \mathrm{PDF}\left(L_n^{\mathrm{f}}, \frac{L_m^{\mathrm{f}}}{2}, S\right), \tag{12}$$

where S is the standard deviation, L_m^{f} the parent fiber length, L_n^{f} the child fiber length and the scaling factor ϱ_m is defined to fulfill the constitutive condition, as described in [8]. The indices n and m represent the number of possible fiber lengths. It is $R_{nm} = R_{(m-n)m}$ since the initial fiber length and one length of a child define the length of the other child. Furthermore, it is $R_{nm} = 0$ for $L_n^{\mathrm{f}} \geq L_m^{\mathrm{f}}$, so short fibers cannot combine to longer fibers again.

Finally, the number of fibers N_n^{f} with corresponding length L_n^{f} within a control volume is given by

$$\frac{\partial N_n^{\mathrm{f}}}{\partial t} + U_i \frac{\partial N_n^{\mathrm{f}}}{\partial x_i} = -P_n N_n^{\mathrm{f}} + \sum_m R_{nm} N_m^{\mathrm{f}}, \tag{13}$$

where U_i is the velocity vector of the regarded cell.

3. Results and discussion

The novel fiber breakage modeling approach is validated with reactive injection molding experiments of a 190 mm × 480 mm rectangular plate with 4 mm thickness as presented in [5, 12]. The material is injected via a 185 mm long cone sprue with a start and end diameter of 9 mm and 15.5 mm, respectively, ending at the plate's center. The machine used for experiments is a KraussMaffei 550/2000 GX injection molding machine equipped with a standard 60 mm thermoset screw. A part of the screw chamber is also considered in the simulation model to enable a better modeling of the initial material state with respect to fiber orientation and fiber length distribution. The simulation model with part of the screw chamber and position of the fiber length measurement is shown in Figure 1. The material enters the cavity in the blue highlighted area.

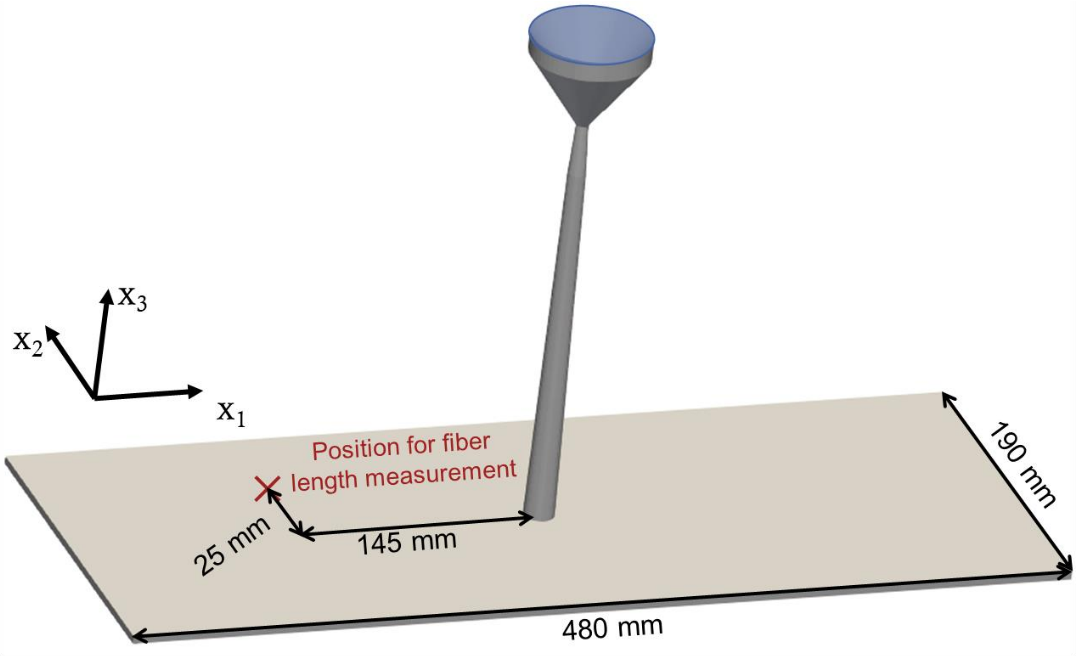

Figure 1. Simulation model for validation with inlet area highlighted in blue

The material used for the experiments is phenolic long-fiber compound of the novolac type, called Porophen GF9201L12a by Sumitomo Bakelite Co., Ltd [13]. The material is reinforced with 55 %-wt. glass fibers, having an initial length of 12 mm. The fiber length measurement is performed with pyrolysis and the commercially available FASEP system by IDM Systems as described in [12].

As shown in [5, 12] only a small amount of fibers remains with a length of 12 mm after plastification (about 5 % by weight). The majority of fibers is already broken to less than 1 mm, being about 75 % in summary. The fiber length distribution after plastification (screw chamber) is shown in Figure 2 by the black, dotted curve. It represents the initial state of the simulation model. The material is injected in the cavity with an injection speed of 150 cm^3/s, the mold has a temperature of 185 °C. The considered fiber lengths in the simulation are 0.25 mm to 11.75 mm in 0.5 mm steps, resulting in 24 possible fiber lengths. The measurements are also clustered in 0.5 mm steps. The simulation is performed with the finite-volume based open-source software OpenFOAM. The simulation method and material models are described in [2, 5]. The model parameters for fiber breakage calculation are given in Table 1. The values for C and S are identical to the ones used by Phelps et al. [8].

Table 1: Parameters used for fiber breakage calculation.

Parameter	Value	Unit
E_f	73	GPa
d_f	$17 \cdot 10^{-6}$	m
C	0.025	-
S	1	-

Figure 2 shows the averaged experimental results of five measurements with corresponding standard deviation for the screw chamber and the plate. As can be seen, only a small amount of fibers with less than 25 % has a length of more than 1 mm after plastification, i.e. in the screw chamber. However, there are some longer fibers with 5-8 mm and about 5 % still have a length of 12 mm. During the injection, nearly all fibers break to lengths of 1 mm or less, as shown by the measurements in blue in Figure 2. The position in the plate, where the specimens were taken, is shown in Figure 1. Comparing the experimental results in the plate (blue) to the simulation results (red) shows a good agreement between simulation and experiments for the complete length distribution. Also in the simulation nearly all fibers break to less than 1 mm and the amounts of fibers with 0.25 mm and 0.75 mm are quite similar in simulation and measurements. The good agreement validates the presented approach to be able to predict reasonable fiber length distributions in injection molding simulation, with respect to process conditions and material properties.

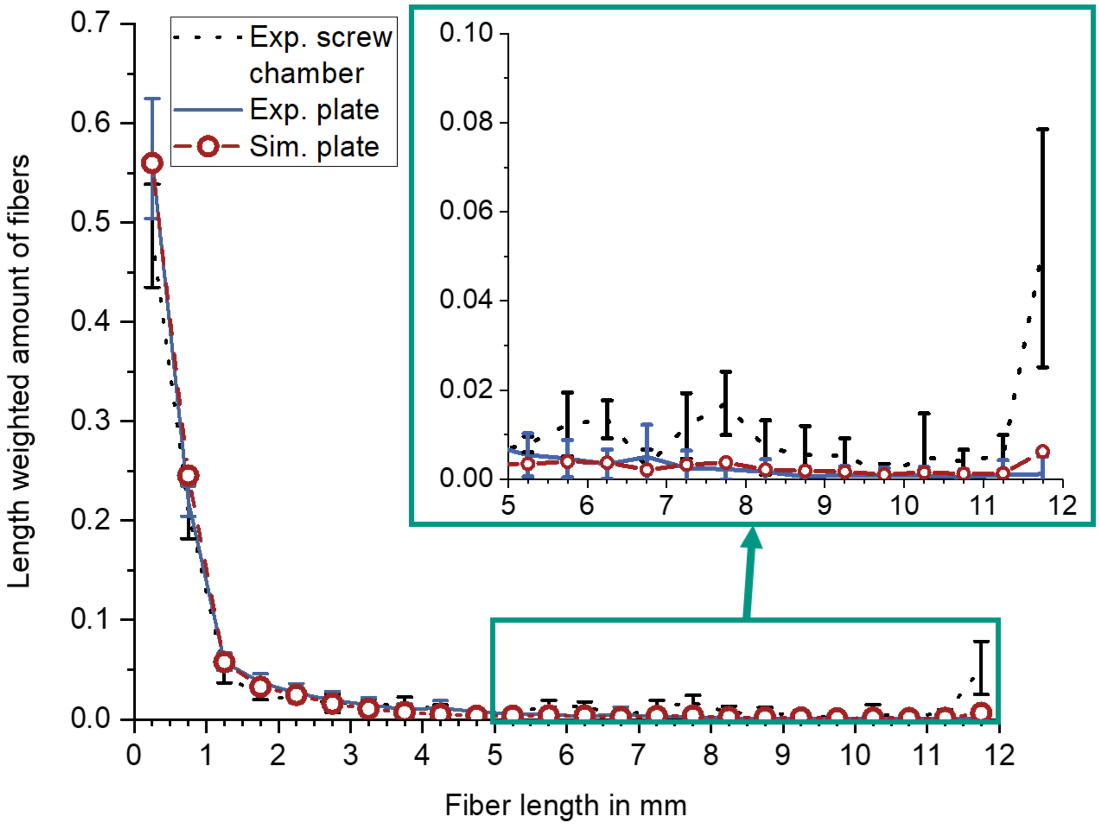

Figure 2. Comparison of fiber length for experimental results in screw chamber (black, dotted), plate (blue, lines) and simulation in plate (red, circles), experimental results are shown with standard deviation

4. Conclusion and outlook

A novel approach for simulation of fiber breakage in macroscopic injection molding simulations is presented. The approach focuses on reference fibers, represented by the eigenvectors of the second order orientation tensor. Hydrodynamic drag and lift force are calculated individually for all eigenvectors. Based on hydrodynamic load and buckling, a constitutive fiber breakage model predicts the fiber length distribution during injection molding with respect to process conditions and material properties. The method is validated with experimental fiber length distribution measurements of an injection molded plate, showing good agreement.

The main difference between this approach and the one presented by Phelps et al. [8] is the procedure of the force calculation, which has two effects. One is that the forces within this work are related to the eigenvectors and hence there are three forces for three representative fibers with different orientations in each cell. Due to different orientation and the weighting with the eigenvalues it is possible that only an amount of fibers within the control volume is able to buckle and break, which increases the orientation dependence of the breakage modeling. The second point is the reduction of empirical parameters, since the calculation of the hydrodynamic forces can be performed without empirical parameters, reducing the necessary parameters from three to two compared to [8].

Hydrodynamic load is not the only effect which may lead to fiber damaging. One other important aspect are fiber contact forces like normal, friction and lubrication forces, as investigated by Meyer et al. [14] in a mesoscopic fiber bundle simulation approach. Such forces are especially relevant for highly filled materials and influence fiber movement, orientation and damaging. However, the exact effects of these forces on the material behavior, particularly on macroscopic scale, are not well understood at this point of time, whether on the experimental side, nor on the numerical. More investigation in fiber-fiber interactions needs to be done to create a better understanding of these phenomena and the influence on material behavior and properties.

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