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Fiber orientation evolution in simple shear flow from a repeatable initial fiber orientation

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ABSTRACT

Experimental fiber evolution data from a rheometer can be used to determine material parameters in fiber orientation models independent from processing flows. The Folgar–Tucker orientation model was demonstrated in simple shear flow to predict distinctly different trends in the orientation evolution depending on the initial fiber orientation. Repeatable fiber orientation evolution data in a simple shear flow was used to determine material parameters in the strain reduction factor (SRF) and reduced strain closure (RSC) orientation models. The SRF and RSC orientation models were tested with different initial fiber orientations created from an injection molded plaque in order to evaluate the orientation model parameters. A stress equation incorporating fiber-fiber interactions was evaluated independently of the fiber orientation models using experimental orientation evolution data with different initial orientations.

1. Introduction

Discontinuous fiber composites are often manufactured by adapting injection or compression molding processes [1]. During the mold filling process, a complex fiber orientation develops within the part which is dictated by the mold geometry and processing conditions. The variations in fiber orientation throughout the part largely influence the degree to which mechanical properties are improved compared to the polymer matrix [2]. Simulating the development of the fiber microstructure during the molding process can then allow for the optimization of mold designs and processing conditions to improve a part's mechanical performance.

Folgar and Tucker [3] provided the first widely used equation to describe the motion of concentrated fibers during flow through the introduction of an isotropic rotary diffusion term. The strain reduction factor (SRF) [4] and the reduced strain closure (RSC) [5] models were developed as empirical modifications to the Folgar–Tucker model to better reflect slower orientation kinetics observed experimentally. Further adaptation of the RSC model has been employed by Phelps et al. [6] to include anisotropic rotary diffusion to account for fiber interactions that are dependent on the fiber orientation state and flow deformation.

The extra stress in a fiber suspension consists of additive contributions of the suspending matrix and fibers and is dependent on the fiber orientation. The fiber contribution has been described by theory for dilute and semi-dilute concentrations [7-9]. For concentrated suspensions, the general form of the Lipscomb et al. [7] stress equation has been fit to experimental stress data from a rheometer [10,11]. Recently proposed stress models have added stresses resulting from fiber-fiber interactions but these models have been subjected to little investigation outside of the authors' original works [12,13].

In order to use fiber orientation models to provide an accurate description of the fiber orientation in a molded part, empirical parameters in the models must be determined. Empirical expressions for the isotropic rotary diffusion term in the Folgar–Tucker model have been fit to numerical simulations [14,15] or to experimental orientation data obtained from injection molded parts [16]. Wang et al. [5] proposed that the empirical parameters in the RSC fiber orientation model could be obtained from the transient rheological response in shear flow using a stress equation that is dependent on fiber orientation. Eberle et al. [10] and Ortman et al. [17] measured fiber orientation during the startup of flow along with transient stress data to provide an additional comparison between stress and orientation model predictions when fitting parameters in the models. The stress predictions using orientation model parameters fit to experimental data did not reflect the measured stress response. Based on their sample preparation procedure, the initial fiber orientation is not well-controlled which is necessary to reliably assess orientation and stress models during the startup of flow [18].

The overlying goal is to obtain unbiased material parameters used in the fiber orientation models from a fundamental flow that

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can then be used to simulate complex molding processes. The purpose of the work presented here is to demonstrate the importance of the initial fiber orientation when extracting material parameters in fiber orientation models from experimental orientation evolution data. The Folgar–Tucker model is used to establish that the orientation evolution is highly dependent on the initial fiber orientation. The SRF and RSC models are used to reflect the slowed orientation kinetics in the experimental orientation data of fibers with a number average fiber length of 0.7 mm. The SRF and RSC orientation models are compared to experimental fiber orientation evolution data with different initial orientations. Lastly, an accurate stress equation could provide the necessary orientation model information without measurements of fiber orientation. A stress equation that includes an additional fiber-fiber interaction term is evaluated based on the fiber orientation evolution data. The information gathered from the well-defined shear flow can be used to determine and validate material parameters in orientation models that can then be applied in the future to complex molding simulations.

2. Fiber orientation equations

The orientation of a single rigid fiber can be described by a unit vector, **p**, parallel to the length of the fiber. Even-order tensors can be used to compactly represent a population of fibers [19]. The second and fourth order orientation tensors are described, respectively, as:

$$\mathbf{A} = \int \mathbf{pp}\,\psi(\mathbf{p})\,\partial\mathbf{p} \quad \mathbf{A}_4 = \int \mathbf{pppp}\,\psi(\mathbf{p})\,\partial\mathbf{p} \tag{1}$$

where ψ is the orientation distribution function.

Evolution equations for the orientation of rigid fibers have been developed in terms of orientation tensors to improve computational efficiency by avoiding calculations of the orientation distribution function. Folgar and Tucker [3] added a phenomenological rotary diffusion term to account for fiber interactions which was modified empirically by Huynh [4] as the SRF model to better reflect slower orientation kinetics:

$$\frac{D\mathbf{A}}{Dt} = \alpha[\mathbf{W}\cdot\mathbf{A} - \mathbf{A}\cdot\mathbf{W} + \xi(\mathbf{D}\cdot\mathbf{A} + \mathbf{A}\cdot\mathbf{D} - 2\mathbf{D}:\mathbf{A}_4) + 2C_I\dot{\gamma}(\mathbf{I} - 3\mathbf{A})] \tag{2}$$

where D/Dt is the material derivative, $\mathbf{W} = (\nabla\mathbf{v}^t - \nabla\mathbf{v})/2$ is the vorticity tensor, $\mathbf{D} = (\nabla\mathbf{v}^t + \nabla\mathbf{v})/2$ is the rate-of-deformation tensor, $\xi = (a_r^2 - 1)/(a_r^2 + 1)$ is the particle shape parameter of an ellipsoid with the aspect ratio, a_r = length/diameter, $\dot{\gamma} = \sqrt{2\mathbf{D}:\mathbf{D}}$ is the magnitude of the rate-of-deformation tensor, **I** is the unit tensor, α is the strain reduction factor ranging from 0 to 1 and C_I is the interaction coefficient. For slender fibers, ξ is often set to one, which also helps alleviate non-physical oscillations when approximating $\mathbf{A}_4$ [5]. When $\alpha = 1$, the Folgar–Tucker model [3] is recovered. The addition of the strain reduction factor causes the model to violate material objectivity, meaning that model predictions could depend on the chosen coordinate system.

Wang et al. [5] addressed material objectivity in the RSC model by empirically scaling the evolution of the eigenvalues of **A** while the rotation rate of the eigenvectors remains unchanged:

$$\frac{D\mathbf{A}}{Dt} = \mathbf{W}\cdot\mathbf{A} - \mathbf{A}\cdot\mathbf{W} + \xi\{\mathbf{D}\cdot\mathbf{A} + \mathbf{A}\cdot\mathbf{D} - 2[\mathbf{A}_4 + (1-\kappa)(\mathbf{L}_4 - \mathbf{M}_4 : \mathbf{A}_4)] : \mathbf{D}\} + 2\kappa C_I\dot{\gamma}(\mathbf{I} - 3\mathbf{A}). \tag{3}$$

The value of κ ranges from 0 to 1. The Folgar–Tucker model is recovered when $\kappa = 1$. The two additional fourth order tensors that arise in the model are:

$$\mathbf{L}_4 = \sum_{i=1}^{3} \lambda_i \mathbf{e}_i\mathbf{e}_i\mathbf{e}_i\mathbf{e}_i \quad \mathbf{M}_4 = \sum_{i=1}^{3} \mathbf{e}_i\mathbf{e}_i\mathbf{e}_i\mathbf{e}_i \tag{4}$$

where λ_i are the eigenvalues and $\mathbf{e}_i$ the eigenvectors of **A**.

A primary focus is given to the evolution of the second order orientation tensor, but theories for the extra stress consider the fourth order orientation tensor [7,20]. In simple shear flow, the A_{1212} component of orientation contributes the shear stress when x_1 is defined as the flow direction with the velocity varying in the x_2 direction. The orientation component, A_{1211} has been shown to be a larger contributor to the first normal stress difference than A_{1222} [21].

3. Fiber orientation measurements

Repeatable fiber orientation data was obtained from 30 wt% glass fiber in a polypropylene matrix subjected to simple shear flow within a sliding plate rheometer [22]. The viscosity of the polypropylene matrix does not change significantly from the zero shear viscosity until a shear rate of at least 10 s^{-1} [23]. Additionally, no significant transient behavior was observed at a shear rate of 1.0 s^{-1}. For the experimental conditions in this work, the matrix can be regarded as a Newtonian fluid. Samples were subjected to the startup of simple shear flow for 100 strain units at a gap thickness of 1.5 mm. The initial fiber orientation was generated from injection molded end-gated plaques. The samples derived from the injection molded plaques measured 238.5 mm in length by 76 mm in width and had a thickness of 1.5 mm. Further details on the molding conditions can be found elsewhere [22]. Flow reversal experiments to generate the initial fiber orientation could not be used because no significant transients in orientation were observed during these tests, which make it impossible to assess the slowdown of fiber orientation [22]. For the homogeneous initial fiber orientations in the flow reversal experiments, the fiber orientation remained homogeneous through the gap width for all strains. In addition, the stress response measured during the flow reversal experiments exhibited poor repeatability. In order to assess the performance of fiber orientation models, experimental orientation data had to have good repeatability and change significantly with strain to minimize any measurement error. These criteria were best met using injection molded plaques to produce the initial fiber orientation for transient shear flow experiments. The purpose of using injection molded parts for the initial fiber orientation in the rheometer is that the injection molding process has a strong repeatable flow profile that will yield a fiber orientation that is repeatable between multiple samples. Fiber orientation within the plaques has been measured to be primarily in-plane, thus minimizing the contribution of fiber-wall interactions [22]. Here, one set of initial fiber orientation data is used, but by varying the injection molding conditions, samples could be produced for the rheometer with different initial fiber orientations. The molding process produced samples with a number average (L_n) and weight average (L_w) fiber length of 0.70 and 0.89 mm, respectively. The fiber lengths averaged through the sample thickness were verified to not change within experimental error from 0 to 75% plaque width. The fiber diameter was measured to be 13.3 µm.

The method of ellipses was used to measure the fiber orientation of samples subjected to simple shear flow in the sliding plate rheometer. A cross section of a sample was polished using metallographic techniques and imaged under an optical microscope at 20× magnification [24]. The rigid particle assumption associated with the method of ellipses and the models in Section 2 was confirmed by an insignificant number of fibers having curvature in the micrographs. The method of Vélez-García et al. [25] was used to determine the in-plane orientation angle unambiguously. The second and fourth order fiber orientation tensors are calculated based on a population of measured fibers and a weighting function to