2-D Simulations of Orientation in Highly Concentrated Short Glass Fiber Thermoplastic Composites Made by Injection Molding

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Abstract
The prediction of orientation for high aspect ratio fiber composites is required in order to optimize the mold design of injection molding composites. At present, commercial simulators for fiber composites can qualitative predict the fiber orientation. Some reasons for the limitations of the predictions are the inexistence of a reliable model to predict concentrated regime of fiber suspension, the use of a decoupled scheme to solve the flow and orientation equations, and the simulations are based on Hele-Shaw flow approximations. In this study, the flow through a center gated disk is simulated numerically for a highly concentrated short glass fiber in a PBT (Newtonian) matrix. The fibers are modeled considering the rotary diffusion term and non-affine motion for fibers. In addition, the parameters used in the orientation evolution and constitutive equation were determined from simple flow experiments. For this, a 2D Finite Element Method analysis was performed using the traditional Galerkin method for the balance equations and discontinuous Galerkin for the constitutive equations. The impact of initial fiber orientation and the impact of the rheologically-obtained parameters were investigated. The predictions were evaluated with experimental data obtained using laser confocal microscopy.

Introduction

Injection molded, short-glass fiber thermoplastic composites are an attractive technology to manufacture lightweight, high performance materials. These composites have excellent properties when the fibers are in a concentrated regime and aligned collinearly to the direction of mechanical interest. However, the fiber orientation varies through the part as a consequence of flow induced orientation during the forming. Then, the anticipation of the fiber orientation is required to optimize of the process. In this paper, a 2D solution for a coupled flow and fiber orientation is developed using the Hele-Shaw (HS) approximation which is the typical method of flow description in commercial simulators. The material behavior is modeled using a modified version of the Folgar-Tucker model, adapted to highly concentrated regime and obtained by well controlled rheological and orientation experiments. The polymeric matrix has a Newtonian behavior.

Governing Equations

The HS flow approximation for an isothermal flow in a center gated disk is described by

$$\frac{1}{r}\frac{\partial}{\partial r}\left(h r \bar{v}_r\right)=0 \tag{1}$$

$$-\frac{\partial p}{\partial r}+2\eta\frac{\partial^2 v_r}{\partial z^2}+\frac{1}{r}\frac{\partial}{\partial r}\left(rT_{rr}\right)+\frac{\partial T_{zr}}{\partial z}-\frac{T_{\theta\theta}}{r}=0 \tag{2}$$

where r represents the radial or flow direction, z the gapwise direction, h the half gap width and $\bar{v}_r$ the average radial velocity along the gapwise coordinate, p the pressure, T_{ij} the fiber-contribution to the extra-stress tensor components. These equations are supplemented by the typical boundary conditions for pressure and velocity.

The hydrodynamic extra-stress model is used to represent the fiber-contribution and is defined as

$$\mathbf{T}=\nu\zeta_{str}\left(\left(\nabla\mathbf{v}\right)^T+\nabla\mathbf{v}\right):\mathbf{AA} \tag{3}$$

where ν represents the fiber concentration, $\mathbf{A}$ the second order orientation tensor, and ζ_{str} the viscous drag coefficient.

The evolution of the second order orientation tensor is governed by:

$$\frac{\partial\mathbf{A}}{\partial t}+\mathbf{v}\bullet\nabla\mathbf{A}=\alpha\Big[\left(\nabla\mathbf{v}\right)^T\bullet\mathbf{A}+\mathbf{A}\bullet\left(\nabla\mathbf{v}\right)-2\left(\left(\nabla\mathbf{v}\right)^T+\nabla\mathbf{v}\right):\mathbf{AA}$$
$$-6C_I II\left(\mathbf{A}-\frac{1}{3}\delta\right)\Big] \tag{4}$$

where α represents the slip parameter, C_I the interaction coefficient and II the magnitude of the rate of deformation tensor. The inter-fiber interactions in a semi-dilute and concentrated regime are represented by the last term[1] and the slip parameter[2] in Eq. (4), respectively. With α=1 and C_I =0, Eq. (4) reduces to the Jeffery model, which only accounts for the kinematic effects typical in dilute suspensions.

Problem Description and Numerical Methods

A 75% short shot center-gated disk of 30wt% short glass fiber PBT with internal radius (r_i) of 2.98

mm, outer radius (R) of 30.81 mm, and thickness ($2h$) of 1.31 mm was simulated. The filling time of the part was approximately 1 s and the injection pressure was estimated to be 20 MPa. The material parameters were determined from steady shear and start-up of shear experiments. Over a wide range of shear rates the PBT matrix behaves like a Newtonian fluid with viscosity η = 426 Pa·s. The fiber parameters were determined as $\alpha = 0.40$, $\nu\zeta_{str} = 7417$ Pa and $C_I = 0.02^2$. The weighted average length of the fiber was 364μm.

The initial orientations of the fibers were experimentally determined at the gate using the method of ellipses[5] from laser confocal micrographs taken on metallographically polished surface in r,z-planes. The samples were cut along a line of constant θ. For validation purposes the orientation was determined in a similar manner along the gapwise direction at 40% and 90% of (R-r_i).

The standard Galerkin method (GFEM) is used in the discretization of the HS flow approximation of the balance equations. The discontinuous Galerkin method (DGFEM) with a standard explicit Euler scheme is used to discretize the evolution equations. In the simulations only the top half of the domain was considered with no slip velocity at the wall and symmetry boundary conditions at z=0.

Results and Discussion

There are a limited number of studies which include both experimental and numerical work, therefore the initial conditions of orientation have typically been assumed as random orientation, especially for a center-gated disk. The orientation determined experimentally from a 75% short shot center-gated disk showed an non-smooth, asymmetric profile at the gate region which corroborates predictions indicted in the literature but never validated[3,4]. Similar asymmetric orientation profile is observed at 40% and 90% (R-r_i). However, simulations using the current and the modified model showed a smooth profile of orientation along the height for those radial locations. The reason for such smooth behavior can be attributed to a fast prediction of steady state. Then the model used in this study can not reproduce the long transient behavior introduced by the inter-particle interactions in highly concentrated fiber suspensions. The predicted transient behavior is seen at very short filling time, then the experimental orientation was compared to this transient orientation. Figure 1 shows the measured orientation at the top half of the gate (magenta lines) and 90% (R-r_i) (red lines) for PBT filled with short glass fiber and the prediction at 90% (R-r_i) using only the Jeffery model with measured orientation values at the gate (blue line). The prediction using measured gate orientation shows several peaks and valleys that can be related to the layered structure formed at the gate which evolves locally as the flow progresses. The predicted profile at 90% (R-r_i) can reproduce at least qualitatively, and in some regions quantitatively, the experimental profile. This is in sharp contrast with predictions using a random orientation at the gate (green line) or a prescribed constant orientation at the gate (not shown) which fail to show the layered structure.

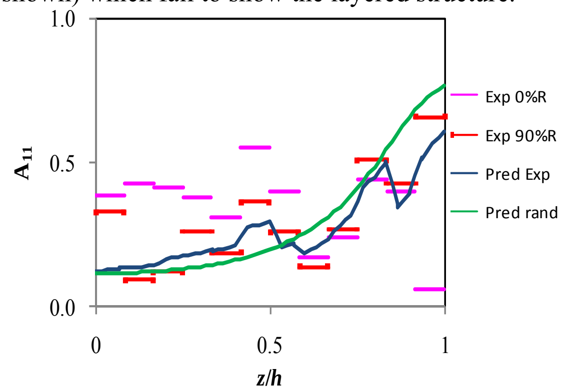

Figure 1. Experimental values of A_{11} at the gate and close to the end of fill (90% of radial flow length) with the predicted values of A_{11} orientation component close to the end of fill using random or measured orientation at the gate.

Conclusion

The impact of inter-particle interactions and the orientation at the gate was investigated using parameters determined from rheometry. When the transient behavior is considered, model predictions are significantly improved by using a localized orientation measured experimentally at the gate region instead of constant orientation assumed in previous studies. The predicted profile in different radial positions can be related to the layered structure along the gapwise direction. Model modifications including interactions have lower impact than the initial conditions.

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