Simulation of Orientation in Injection Molding of High Aspect Ratio Particle Thermoplastic Composites

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Abstract. A 2D coupled Hele-Shaw flow approximation for predicting the flow-induced orientation of high aspect ratio particles in injection molded composite parts is presented. For a highly concentrated short glass fiber PBT suspension, the impact of inter-particle interactions and the orientation at the gate is investigated for a center-gated disk using material parameters determined from rheometry. Experimental orientation is determined from confocal laser micrographs using the methods of ellipses. The constitutive equations are discretized using discontinuous Galerkin Finite Elements. Model predictions are significantly improved by using a localized orientation measured experimentally at the gate region instead of random or averaged gapwise measured 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.

Keywords: Fiber suspensions; Hele-Shaw approximation; DGFEM; Coupling effect; Injection molding; Composites

INTRODUCTION

High aspect ratio particle reinforced thermoplastics made by injection molding are an attractive technology to develop lightweight, high-performance materials. The desired properties are only obtained when the particle orientation is in the direction of mechanical interest. However, the particle orientation varies through the part as a consequence of flow induced orientation during the forming. The high aspect ratio particles considered here are short glass fibers and nanoparticles, but the focus will be on the former because there are reliable methods to evaluate their orientation experimentally. 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 Doi model for particles combined with either a Newtonian or viscoelastic model for the polymer matrix.

GOVERNING EQUATIONS

The HS flow approximation can be used to approximate the conservation equations for molds with a thickness much smaller than the overall part dimension. Isothermal flow in a center gated disk is then described by the following modified mass balance and momentum equations, respectively

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

$$-\frac{\partial p}{\partial r}+\frac{\partial T_{rz}}{\partial z}=0 \tag{2}$$

where r represents the radial or flow direction, z the gapwise direction, h the half gap width and $\overline{v}_r$ the average radial velocity along the gapwise coordinate, p the pressure, T_{rz} the shear component of the extra-stress tensor. These equations are supplemented by the typical boundary conditions for pressure and velocity[1]. The flow is assumed to be symmetrical in angular direction, θ.

The model used for the extra-stress tensor for a high aspect ratio particle-filled polymeric suspension consists of various components

$$\mathbf{T} = \mathbf{T}^{matrix} + \mathbf{T}^{particles} \tag{3}$$

$$\mathbf{T}^{particles} = \left(\nu k_B T/2\underline{D}_r\right)\mathbf{F}\left(\mathbf{A}\right) + \nu\zeta_{str}\left(\left(\nabla\mathbf{v}\right)^T + \nabla\mathbf{v}\right) : \mathbf{AA} \tag{4}$$

$$\mathbf{F}\left(\mathbf{A}\right) = -6\bar{D}_r\left(\left(\mathbf{A} - \frac{1}{3}\delta\right) + U\left(\left(\mathbf{A}\bullet\mathbf{A}\right) - \left(\mathbf{A}:\mathbf{A}\right)\mathbf{A}\right)\right) \tag{5}$$

where $\mathbf{T}^{matrix}$ represents the extra-stress tensor contribution due to the matrix, assumed as a viscous fluid and $\mathbf{T}^{particles}$ the extra stress contributions due to the particles. The particle stress has a Brownian and hydrodynamic component represented by the first and second term in Eq. (4), respectively. In Eq. (4) ν represents the particle concentration, k_B the Boltzmann constant, T the absolute temperature, $\bar{D}_r$ the average rotational diffusivity in a concentrated system due to constraints of neighbor rods, **A** the second order orientation tensor, and ζ_{str} the viscous drag coefficient which is typically described by the Dinh and Armstrong model[2]. **F**(**A**) is the Brownian contribution defined by the Doi model[3], with U representing the interaction potential for a concentrated suspension. The Brownian term is relevant for high aspect ratio particles less than 10μm such as nanoparticles; for non-Brownian particles such as short glass fibers this term can be neglected.

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

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

where C_I, represent the interaction coefficient and II the magnitude of the rate of deformation tensor. **F**(**A**) represents the Brownian contribution as described in the Doi model[3], and the last term represents the Brownian like term accounting for inter-particle interactions for non-Brownian particles introduced by Folgar and Tucker[4]. With **F**(**A**)=**0** and C_I =0, Eq. (6) 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 = 350 Pa·s. The particle parameters were determined as $\nu\zeta_{\mathrm{str}}$ = 7417 Pa and C_I = 0.001. The weighted average length of the fiber was 500μm therefore Brownian contributions can be neglected (**F**(**A**) = **0**).

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. The initial orientation tensor **A** was computed using a weighted average of orientations of all individual particles within rectangles of dimension $h/12$ in z-direction and $h/3$ in r-direction. 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.

NUMERICAL RESULTS AND DISCUSSION

There are a limited number of studies including a simultaneous experimental and numerical program, 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 asymmetric profile at the gate region which corroborates predictions indicted in the literature but never validated[6,7]. Figure 1a 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. These two gate orientations are always used in injection molding simulations and result in similar orientation profiles. All simulations fail to predict the measured orientation for the segment next to the axis of symmetry, the reason for this needs further investigation. The results from the simulations for A_{11} component using piecewise initial orientation suggest a fading effect of the initial multilayered structure forming at least a shell-transition-core layer structure at long radial distances from the gate, as illustrated in Figure 1.b. Similar has been observed the other dominant orientation component, A_{33}. The inter-particle interactions through the Folgar-Tucker term (C_I=0.001) was considered in the model to try to improve predictions obtained with the Jeffery model. However, the predictions using the additional terms with experimental piecewise initial orientation produced only slight changes in the predicted orientation, almost overlapping the predictions obtained using the Jeffery model. Increasing the value of C_I to values in the range of 0.016 to 0.003, commonly found in the literature[4,8], also did not significantly change the orientation predictions.

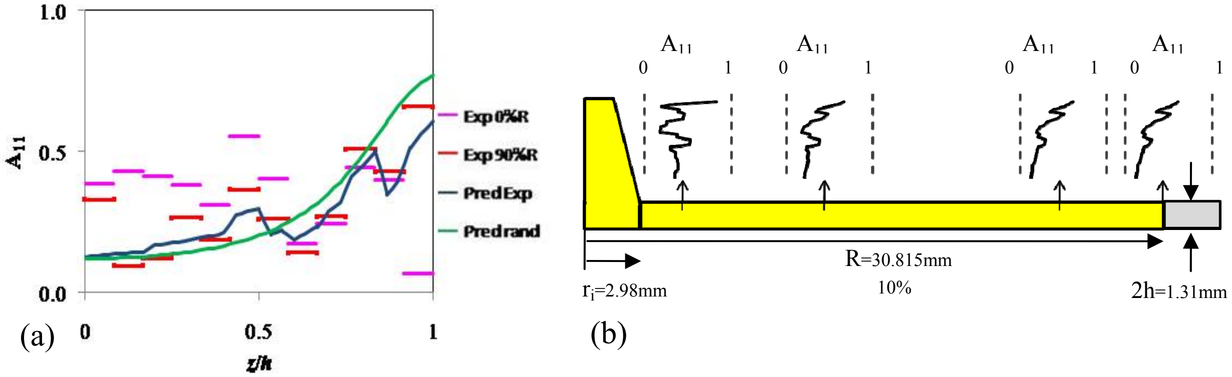

FIGURE 1. (a) Experimental values of A_{11} at the gate and close to the end of fill (90% of radial flow length) with the predicted values of A_{11} orientation component close to the end of fill using random or measured orientation at the gate. (b) Evolution of orientation in a 75% short shot showing a layered structure expressed through the predicted A_{11} profiles at several locations in the top half of the disk.

CONCLUSIONS

A 2D coupled method for predicting the flow-induced orientation of high aspect ratio particles in thin walled injection molded composite parts has been presented. The impact of inter-particle interactions and the orientation at the gate was investigated using parameters determined from rheometry. Model predictions are significantly improved by using a localized orientation measured experimentally at the gate region instead of random or averaged gapwise measured 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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