SIMULATION OF ORIENTATION IN INJECTION MOLDING OF A HIGHLY CONCENTRATED, SHORT GLASS FIBER THERMOPLASTIC COMPOSITES

Gregorio M. Vélez-García, Kevin Ortman, Aaron P.R. Eberle, Peter Wapperom, and Donald G. Baird,
Virginia Tech, Blacksburg, VA

Abstract

This paper presents a 2D coupled Hele-Shaw flow approximation for predicting the flow-induced orientation of injection molded composite parts within a commercial concentration range. 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 a time-delayed orientation evolution equation and their material parameters determined from rheometry. Experimental orientation at the gate and at several radial positions in the cavity is determined using the method of ellipses. The orientation evolution 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 orientation assumed in previous studies. Model modifications, orientation at the gate, and coupled simulations are required to improve the prediction of the fiber orientation.

Introduction

Fiber reinforced thermoplastic made by injection molding is an attractive technology to develop lightweight, high-performance materials. The lightweight molded composites consist of a polymeric matrix reinforced with fibers because of the excellent mechanical properties obtained in the final product, the high throughput, and the cost reduction. The desired properties are only obtained when the orientations of the particles in the direction of mechanical interest are met. However, the fiber orientation varies through the part as a consequence of flow within the mold during the forming; a concept called flow induce orientation. The fibers considered here are short glass fiber defined as fiber with high aspect ratio ($a_r > 30$) and absolute length below 1 mm.

Optimization of the technology requires a prediction tool using a computer model capable of designing the correct molding machinery, molding and processing conditions, and consistently controlling fiber orientation. The actual capabilities of simulations are unable to make a quantitative prediction of the orientation due to several limitations in the modeling and numerical techniques used to solve the system of equations. Some of these limitations are the use of models which ignore the fiber interactions (Jeffery model), or account for them in a concentration below the commercial interest (Folgar-Tucker model), or ignore the viscoelastic effects of the polymer, and use a decoupled approach to solve the system of equations.

This paper develops a 2D solution for a coupled flow and fiber orientation using the Hele-Shaw approximation, which is the typical method of flow description in commercial simulators. The material behavior is modeled using the Eberle-Baird-Wapperom-Vélez[1] (EBWV model) and a Newtonian model for the polymer matrix, with parameters determined from simple flow rheology. The EBWV is a modified version of Folgar-Tucker[2] model for highly concentrated fiber suspension. The objective of this work is to develop an accurate numerical tool capable of predicting the flow-induced orientation of glass fiber in a commercial range of concentrations using a coupled approach.

Theoretical Background

Balance Equations

The conservation equations for isothermal flow and highly viscous fluid are described by

$$\underline{\nabla} \bullet \underline{v} = 0 \tag{1}$$

$$\underline{\nabla} \bullet \left(-p\underline{\underline{\delta}} + \underline{\underline{T}} \right) = \underline{0} \tag{2}$$

where $\underline{\nabla}$ represents the gradient operator, $\underline{v}$ the velocity, p the pressure, $\underline{\underline{\delta}}$ the identity matrix, and $\underline{\underline{T}}$ the extra stress tensor. The lubrication approximation can be used to simplify the conservation equation based on the fact that the molded parts thickness is less than the overall part dimension. The simplified equation is known as Hele-Shaw flow approximation. When a center-gated disk geometry as shown in Figure 1 is considered, the Hele-Shaw flow approximation is described by

$$\frac{1}{r}\frac{\partial}{\partial r}\left(hr\overline{v}_r \right) = 0 \tag{3}$$

$$-\frac{\partial p}{\partial r} + \frac{\partial T_{rz}}{\partial z} = 0 \tag{4}$$

where r represents the radial or flow direction, z the gapwise direction, h the half gap width, $\overline{v}_r$ the average radial velocity along the gapwise coordinate, p the pressure, and T_{rz} the shear component of the extra-stress tensor. These equations are supplemented by the typical boundary conditions for pressure and velocity[3]. The flow is assumed to be symmetrical in the angular direction, θ.

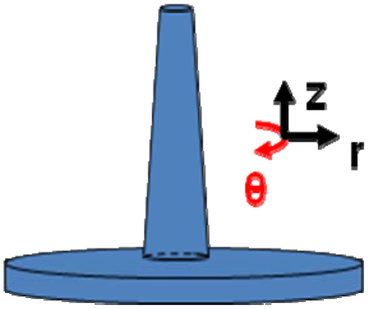

Figure 1. Center-gated disk geometry.

Orientation Equation

The orientation evolution tensor described by EBWV model combines the Jeffery model, Folgar-Tucker term, and a non-affine motion behavior. The non-deviatoric form of the model in a Newtonian solvent is described by

$$\frac{D\underline{\underline{A}}}{Dt}=\frac{\partial\underline{\underline{A}}}{\partial t}+\underline{v}\bullet\underline{\nabla}\underline{\underline{A}}=\alpha\left[\underline{\underline{G}}\left(\underline{\underline{A}},\underline{\underline{\kappa}}\right)+\underline{\underline{FT}}\left(\underline{\underline{A}}\right)\right] \tag{5}$$

$$\underline{\underline{G}}\left(\underline{\underline{A}},\underline{\nabla}\underline{v}\right)=\underline{\nabla}\underline{v}^{T}\bullet\underline{\underline{A}}+\underline{\underline{A}}\bullet\underline{\nabla}\underline{v}-2\underline{\underline{d}}:R_4 \tag{6}$$

$$\underline{\underline{FT}}\left(\underline{\underline{A}}\right)=-6C_I II\left(\underline{\underline{A}}-\frac{1}{3}\underline{\underline{\delta}}\right) \tag{7}$$

where $\underline{\underline{A}}$ and R_4 represent the second order and fourth non-deviatoric orientation tensors, respectively. $\underline{\underline{G}}(\underline{\underline{A}},\underline{\nabla}\,\underline{v})$ and $\underline{\underline{FT}}(\underline{\underline{A}})$ denote the kinematic and semi-dilute-regime interaction contributions to the orientation, respectively. α is the non-affine constant, which is a time-delayed constant used to describe the multi-particle interactions in a concentrated suspension seen as a slowing down process of orientation. C_I is the interaction coefficient, II the magnitude of the rate of deformation tensor, and $\underline{\underline{d}}$ the rate of deformation tensor. R_4 can be expressed in terms of a quadratic closure

$$R_4=\underline{\underline{A}}\,\underline{\underline{A}} \tag{8}$$

The EVWB model described by Eq. (5) is a non-objective model but the simplification introduced by the Hele-Shaw approximation allows us to use the model to predict the flow-induced orientation in the center-gated disk flow[4].

The initial conditions for the experimentally measured orientations at the gate of the part are used for the proposed model for fiber orientation. The orientation is measured using confocal laser or optical-reflection microscopy.

Constitutive Equations

The extra stress tensor for a fiber-filled polymeric suspension consists of various components

$$\underline{\underline{T}}=\underline{\underline{T}}^{fibers}+\underline{\underline{T}}^{matrix} \tag{9}$$

where $\underline{\underline{T}}^{fibers}$ is the stress due to the movement of short glass fibers in the fluid and $\underline{\underline{T}}^{matrix}$ is the contribution of the polymer matrix. The extra stress tensor contribution due to the matrix depends on the behavior of the polymer used as solvent. For matrices behaving like a Newtonian fluid, the Newtonian constitutive equation can be used to describe the polymer. It has the form

$$\underline{\underline{T}}^{Matrix}=2\eta\underline{\underline{d}} \tag{10}$$

where η is the Newtonian viscosity. The extra stress contribution of the short glass fibers can be modeled

$$\underline{\underline{T}}^{fibers}=\nu\zeta_{str}\underline{\underline{d}}:\underline{\underline{\underline{\underline{A}}}} \tag{11}$$

where ν denotes the particle concentration. ζ_{str} represents the viscous drag coefficient, typically described by the Dihn and Armstrong[5] model in the form

$$\zeta_{str}=\frac{\pi\eta_s l^3}{12\ln\left(2\,{}^{h}\!/_{d}\right)} \tag{12}$$

Problem Description

A 75% short shot center-gated disk of 30 wt% 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 particle parameters were determined as $\nu\zeta_{str}$ = 5000 Pa⋅s and C_I = 0.02. The weighted average length of the fiber was 364 μm.

The initial orientations of the fibers were experimentally determined at the gate using the method of ellipses[6] from laser confocal or optical-reflection micrographs taken on a 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).

Numerical Methods

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.

Discussion

Experimental orientation

A limited amount of studies exist in the literature including a simultaneous experimental and numerical program. They typically assume random initial orientation conditions along the thickness, especially for a center-gated disk. That means a plug-like profile for the major orientation component as shown in Figure 2(a). However, the orientation determined experimentally from a 75% short shot center-gated disk showed in Figure 2(b) reveals an asymmetric profile at the gate region. This result corroborates predictions indicted in the literature but never validated[7,8]. The experimental results in Figure 2(b) also show that the values of orientation components are far from random orientation, especially for the A_{zz} components.

The orientation along the thickness measured at 40% and 90% (R-r_i) for PBT filled with short glass fiber indicates changes in the magnitude and distribution of the orientation components compared to the orientation at the gate. Figure 3 shows the experimental evolution of the orientation for the A_{rr} orientation components in the gate, 40% and 90% (R-r_i). The initial asymmetry fades as the function of the radial location, but still is present at regions close to the end of flow for the size of center-gated disk used in the experiments. However, the experimental results suggest the development of a symmetric orientation or stable structure of orientation for disks of larger diameter as described by Rao and Altan[9].

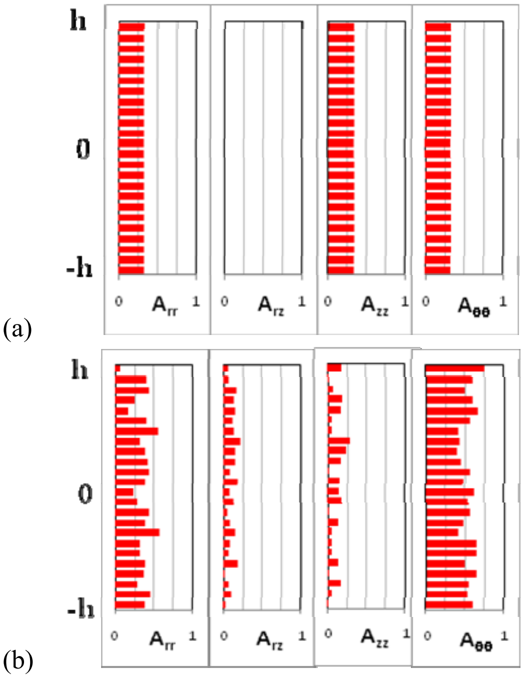

Figure 2. Experimental values of A_{ij} along the cavity thickness at the (a) gate and (b) close to the end of fill (90% of radial flow length).

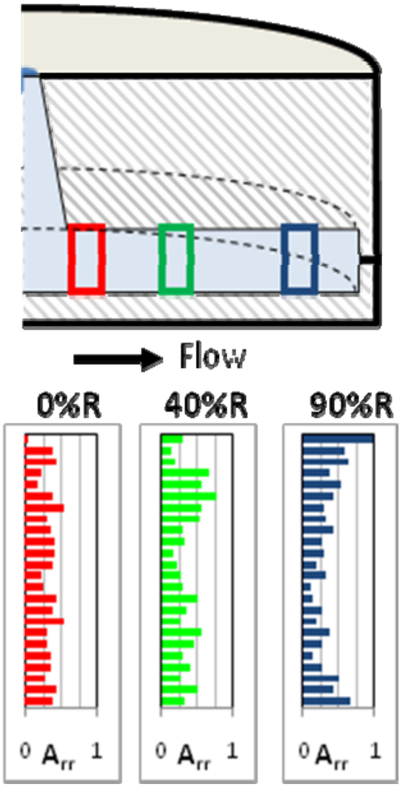

Figure 3. Experimental values of A_{rr} along the cavity thickness at three radial locations: gate, 40% (R-r_i), and 90% (R-r_i).

Prediction of orientation

The predicted evolution of orientation in the cavity is influenced by the asymmetric orientation at the gate and the simulation strategy, i.e, coupled or decoupled approach. Indeed, the initial orientation affects local values of orientation while the solution strategy affects the velocity of orientation evolution prediction. Figure 4 (a) and (b) shows decoupled simulations results for the radial locations of 40% and 90% (R-r_i), respectively, focused on the upper half cavity at a dimensionless simulation time of 290. These predictions (lines) overestimate the A_{rr} orientation components while they underestimate the $A_{\theta\theta}$ and A_{rz} orientation components, when compared to the experimental results (symbols). The smooth predicted profile can not reproduce a series of peaks and valleys observed in the experimental profile of orientation. These features in the orientation profile can be related to the layered structure formed at the gate, which evolves locally as the flow progresses[10]. However, when the experimental orientation profile is compared with simulation results at a dimensionless simulation time of 2.90 (1% of the simulation time), the values and features of orientation are successfully reproduced. This implies that the decoupled simulation using the EVWB model is evolving faster than the experimental evolution of orientation.

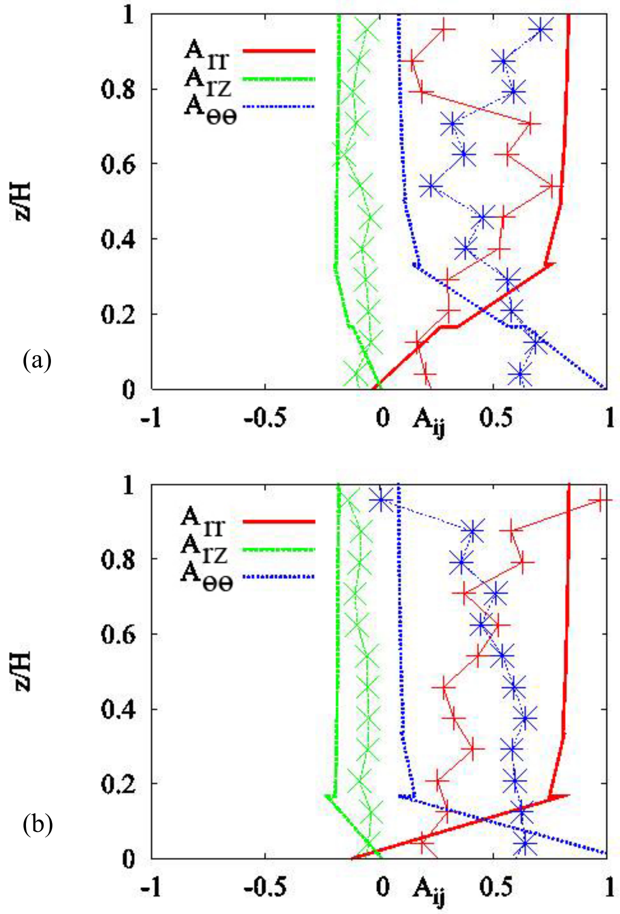

Figure 4. Experimental and predicted orientations from decoupled simulation at (a) 40% (R-r_i) , and (b) 90% (R-r_i) at a dimensionless time of 290. The lines denote the predictions, while the symbols are used to indicate the experimental results.

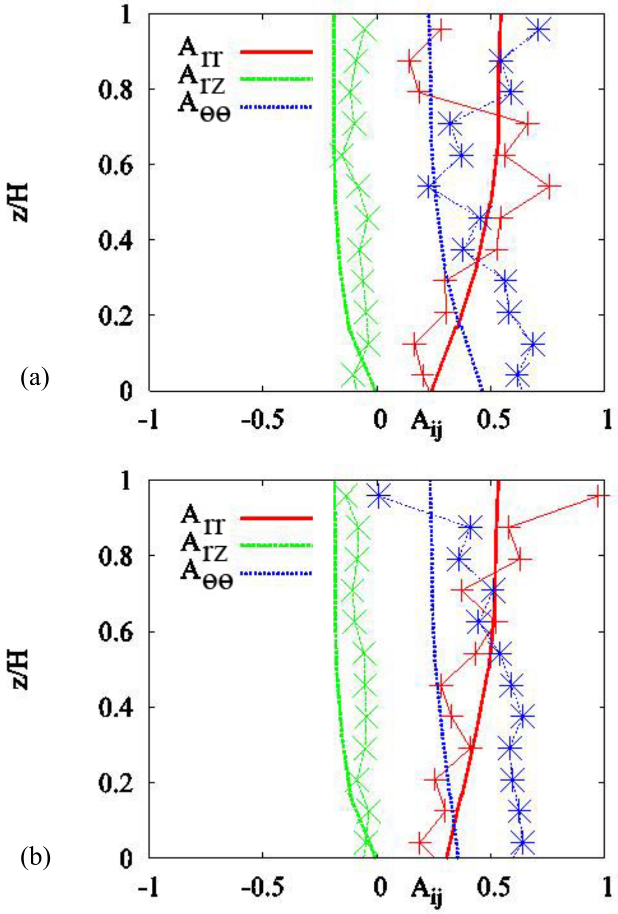

Figure 5. Experimental and predicted orientations from coupled simulation at (a) 40% (R-r_i) , and (b) 90% (R-r_i) at a dimensionless time of 290. The lines denote the predictions, while the symbols are used to indicate the experimental results.

The results of the coupled simulation show improvement in the prediction of the orientation profile. Figure 5 depicts the upper half of the orientation profile at a dimensionless time of 270 for (a) 40% (R-r_i) , and (b) 90% (R-r_i). The results are sensitive to the use of the EBWV model because the retardation of evolution considerably improves the prediction of A_{rr}, but the profile of the predicted orientation is smooth. In general the $A_{\theta\theta}$ is under estimated, but not as severely as in decoupled approach. An interesting observation in coupled simulations is that the difference between experimental and predicted $A_{\theta\theta}$ is greater at 90% (R-r_i) than at 40% (R-r_i). This can be an effect of using the Hele-Shaw approximation, because this simplification ignores the existence of the flow front. It is well known that the front is a region dominated by extensional flow which is the driving mechanism for $A_{\theta\theta}$. Therefore, these coupled results suggest the need for full simulations, which are especially important in small geometries where the evolution of orientation never reaches the stable structure of orientation.

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. Our experimental results indicate that the profile of orientation at the gate can not be assumed as random orientation for a center-gated disk. In addition, the orientation transient remains through the geometry. In the simulation section, the results indicate that the model is not able to retard the orientation evolution in decoupled simulations. However, the coupled simulations improve the prediction of A_{rr} components and suggest the need for simulations considering the frontal flow region.

Acknowledgements

The financial support of NSF/DOE: DMI-052918 is gratefully acknowledged. Gregorio M. Vélez-García also acknowledges support from MS&IE-IGERT, University of Puerto Rico-Mayagüez. The authors also would like to thank the undergraduate student Eric B. Webb, who contributed to the experimental portion of this study.

References

1. A. P. R. Eberle, D. G. Baird, P. Wapperom, and G. M.Velez-Garcia, "Using Transient Rheology to Determine Material Parameters in Fiber Suspension Theory", J. Rheol., submitted
2. F. P. Folgar and C. L. Tucker, *J Reinf Plast Comp* **3**, 98-119 (1984).
3. D. G. Baird and D. I. Collias, *Polymer Processing*, Boston: Butterworth-Heinemann, 1998.
4. Personal communication with Dr Charles Tucker. (2008).
5. S. M. Dinh and R. C. Armstrong, *J Rheol*, **28**, 207-227 (1984).
6. R. S. Bay and C. L. Tucker, *Polym Eng Sci* **39**, 240-253 (1995).
7. B. E. VerWeyst and C. L. Tucker, *Can J Chem Eng* **80**, 1093-1106 (2002).
8. D. H. Chung and T. H. Kwon, *J Non-Newtonian Fluid Mech* **107**, 67-96 (2002).
9. B. N. Rao and M. C. Altan, *J Rheol* **32**, 581-599 (1992).
10. G. M. Vélez-García, K. C. Ortman, A. P.R. Eberle, P. Wapperom, and D. G. Baird "Simulation of Orientation in Injection Molding of High Aspect Ratio Particle Thermoplastic Composites", *Proceedings of the XVth International Congress of Rheology*, Monterey, California, 3-8 August 2008.

Key Words: Fiber suspensions; Hele-Shaw approximation; DGFEM; Coupling effect; Injection molding; Composites.