Long glass fiber orientation in thermoplastic composites using a model that accounts for the flexibility of the fibers

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Abstract

Mechanical properties of long glass fiber composites, used in various industrial applications, are dependant upon the fiber orientation within the part. To date, however, simulations with the ability to predict fiber orientation as a function of mold design are not available. In this study, several options are explored to predict the orientation of long glass fibers in the concentrated regime that take the flexible nature of these fibers into account. Flow through a center gated disk geometry is simulated numerically for high concentrations of long glass fiber in a polypropylene (PP) matrix. For this, a 2D finite element (FEM) analysis was performed using the traditional Galerkin method for the balance equations and the discontinuous Galerkin method for the constitutive equations. Numerical results based on the Hele-Shaw approximation are compared with experiment to verify the models.

Introduction

In an effort to produce lightweight energy efficient parts with high moduli, thermoplastics are reinforced with fibers to increase their stiffness, strength, and impact toughness. Such fibers of interest, within this research, are long glass fibers. Currently, long glass fibers provide a relatively inexpensive means of producing high strength materials used in energy demanding structures such as automobiles, buildings, and aircraft⁴. Additionally, long glass fibers provide much higher properties in the finished part compared to the same part manufactured with short glass fibers, and are therefore the focus of this research. Here the term "long" will be reserved for fibers whose length is greater than or equal to 1mm. In order to obtain parts with optimum mechanical properties, it is desired to predict fiber orientation and configuration as a function of mold design and processing conditions. Hence, the goal of this work is to develop such a simulation scheme.

Much work has been accomplished in simulating the € orientation of short glass fibers in polymeric melts, however relatively few efforts have produced applicable models that can be efficiently used to model long glass fiber orientation. This is, in part, due to the flexible nature of the long glass fibers, whereas short fibers are usually assumed to be rigid. In this research, we explore several models that take

the semi-flexible nature of long glass fibers into affect, and then compare them to experimentally determined results.

Numerical

The Hele-Shaw flow approximation can be used to approximate the momentum equations for molds with a thickness that is much smaller than the length of the overall part. The following simplified form of the continuity and momentum equations, respectively, then describes isothermal flow in a center-gated $disk¹$,

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

$$
-\frac{\partial P}{\partial r} + \frac{\partial T_{rz}}{\partial z} = 0
$$
 (2)

where *r* represents the radial flow direction, *z* the thickness direction, *h* the half gap width and \bar{v}_r

Explicat boundary conditions for pressure and velocity¹. The flow is assumed to be symmetrical in the average radial velocity along the coordinate, *p* the pressure, *Trz* the shear component of the extra-stress tensor. These equations are supplemented by the typical boundary conditions for pressure and angular direction, *θ*.

Several orientation models will be implemented uncoupled from the previous Hele-Shaw form of the equations of change. One such model, which tries to capture the semi-flexible nature of long glass fibers, is given by an extension the Folgar-Tucker equation²,

$$
\frac{DA}{Dt} = \alpha \bigg[(\nabla \mathbf{v})^T \cdot \mathbf{A} + \mathbf{A} \cdot (\nabla \mathbf{v}) - 2 ((\nabla \mathbf{v})^T + (\nabla \mathbf{v})) : \mathbf{A}_4 - 6C_I II \bigg(\mathbf{A} - \frac{1}{3} \delta \bigg) \bigg]
$$
(3)

where A and A_4 are the second and fourth order orientation tensors, respectively, C_I is the Folgar-Tucker constant, II is the magnitude of the rate of strain tensor, and α is a non-affine motion parameter. Note, this equation neglects affects due to Brownian motion as its contributions to the present fibers of interest, based on their dimensions, are negligible. Strautins and Latz proposed another model that will be analyzed⁶. This model accounts for semiflexibility by given the fiber a two-segment, 3-bead representation.

Figure 1. A two-rod model of an elastic fiber. The bending potential depends on the angle θ between the two unit vectors **p**, **q**.

The model is given by the following system of equations,

$$
\frac{DA}{Dt} = \mathbf{A} \cdot \mathbf{\kappa}^T + \mathbf{\kappa} \cdot \mathbf{A} - [(\mathbf{\kappa} + \mathbf{\kappa}^T) \cdot \mathbf{A}] \mathbf{A} + \frac{l_g}{2} [C\mathbf{\mu} + \mathbf{\mu}C - 2(\mathbf{\mu} \cdot C)\mathbf{A}] - 2k[\mathbf{B} - \mathbf{A}(B_{11} + B_{22} + B_{33})] \tag{4}
$$

$$
\frac{DB}{Dt} = \mathbf{B} \cdot \mathbf{\kappa}^T + \mathbf{\kappa} \cdot \mathbf{B} - [(\mathbf{\kappa} + \mathbf{\kappa}^T) \cdot \mathbf{A}] \mathbf{B} + \frac{l_B}{2} [\mathbf{C} \mathbf{\mu} + \mathbf{\mu} \mathbf{C} - 2(\mathbf{\mu} \cdot \mathbf{C}) \mathbf{B}] - 2k[\mathbf{A} - \mathbf{B} (B_{11} + B_{22} + B_{33})] \tag{5}
$$

$$
\frac{D\mathbf{C}}{Dt} = \mathbf{\mathbf{K}} \cdot \mathbf{C} - (\mathbf{A} \cdot \mathbf{\mathbf{K}}) \mathbf{C} + \frac{l_B}{2} (\mathbf{\mu} - \mathbf{C}(\mathbf{\mu} \cdot \mathbf{C})) - k \mathbf{C} [1 - (B_{11} + B_{22} + B_{33})]
$$
(6)

$$
\mu_i = \frac{\partial^2 v_i}{\partial x_i \partial x_k} A_{jk} \tag{7}
$$

where **A** represents the second order orientation tenor, **B** represent the second moment of the dyadic product of **p** and **q** with the orientation distribution function, **C** represents the first moment of the **p** vector with the orientation distribution function, l_B is the segment length, and κ is a value related to the bending rigidity.

The predictions of the preceding models were compared to experimental results. Seventy-five percent short shot center-gated disk of 40wt% long glass fiber in polypropylene matrix with internal radius (*ri*) of 2.98 mm, outer radius (*R*) of 30.81 mm, and thickness (2*h*) 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 experiments⁵. The disks were analyzed with the method of ellipses³ from optical micrographs taken on metallographically polished surface in r,z-planes.

Results and Discussion

Experimental result show that fibers in excess of at least 1 mm show flexibility, thus requiring an orientation model which accounts for it. Numerical results including the affine motion show a behavior which delays the time to which a steady orientation is obtained, as compared to the Folgar-Tucker model. While this behavior is more true to what is determined experimentally, the model possesses objectivity issues. The bead and rod model suggested by Strautins and Latz shows similar dynamic behavior, however values associated with the bending rigidity of the rods have not been verified.

Conclusion

It was found that using experimentally determined initial orientations in the simulation of flow through a center gated disk provided results more true to what was determined experimentally, as opposed to simply assuming initial random orientation. Results predicted using the models of interest were not able to provide quantitative agreement with experiment over the entire flow field, however do begin to qualitatively capture the flexible nature of the long fiber reinforced melts.

Acknowledgments

Financial of NSF/DOE: DMI-052918

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