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PREDICTION OF STIFFNESS FROM ORIENTATION DATA OF GLASS REINFORCED INJECTION MOLDINGS

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Abstract

The complex thermo-mechanical process developing in injection molding leads to through-thickness and point to point variation of fiber orientation. It is not economically viable to characterize experimentally the variation of fiber orientation. Thus, efforts have been put into modeling the fiber orientation in injection molding. Some commercially available programs already allow the prediction of fiber orientation distribution in moldings.

If the fiber orientation field is known it is possible to calculate the major elastic properties, which can be input into finite-element structural analysis codes to predict product performance.

That approach was followed in this work to compare the experimental flexure behavior of glass fiber reinforced polycarbonate injection molded discs with predictions obtained from FEM simulations. The data used in the FEM code was calculated from the fiber orientation data predicted using the software C-Mold.

Introduction

Two main topics are of current interest in the study of processing-morphology-properties of short glass fiber reinforced injection molded thermoplastics: the modeling and measurement of fiber orientation distribution, and the measurement and prediction of mechanical properties of the composites. In both cases, the distribution of fiber orientation plays an essential role.

The earliest work on modeling was done by Jeffery [1], who established the basis of the motion of single ellipsoidal particles immersed in a viscous fluid. It was experimentally verified that in shearing flows the particles tend to align in the direction of the flow. In the case of stretching flows, the fibers tend to align in the direction of the maximum stretching. That direction of stretching is not necessarily the flow direction. In the case of radial and divergent flow, at a position far enough from the injection point, the direction of maximum stretching is perpendicular to the flow and the fibers tend to align in that direction.

Recent research attempted to overcome the difficulties in predicting fiber-fiber interactions during flow, applying some phenomenological parameters to the Jeffery's theory [2-4]. To date no complete theory is available to predict the fiber orientation resulting from the injection molding process. Nevertheless, some models allow the study of the rheological and mechanical properties of short fiber reinforced injection molded composites [5].

It is common in modeling the flow of injection molded composites to consider the fiber orientation evolution as decoupled from the flow simulation. Consequently, the fiber orientation does not affect the flow dynamics or the material viscosity. For concentrated suspensions this simplification can lead to important prediction errors.

The moduli of fiber composites can be estimated from description of the morphology and the properties of the constituents. For systems with regular organization and continuous fibers, the elastic constants can be computed using the rule of mixtures. However, most of the heterogeneous systems, like those developed for injection molding, fall outside those conditions. The characterization of their morphology can only be made in terms of statistical probabilities.

The prediction of the mechanical properties of discontinuous short fiber reinforced composites is made using the principles of composite micromechanics. Halpin et al. [6,7] developed an interpolation procedure that approximates the solutions of the micromechanics theory. The calculation is done with a simple expression that contains an adjustment factor that allows the calculation of the various elastic parameters.

The most typical loading situation for plate moldings is bending. The stiffness of center gated disks, as a paradigm of injection molded plates, can be experimentally determined using a flexure test devised to overcome their inherent non-flatness [8]. This test with three point support and center applied load has been used to characterize the influence of molding conditions on the flexural behavior of the disks.

The flexure test was modeled in a FEM package using quadrilateral composite elements. Those elements allowed the introduction of through-thickness layer properties, as well as along their flow-path variation. The properties that

were calculated after an orientation averaging procedure were input into the FEM program.

The experimental flexure results were compared with the results from the FEM structural simulation.

Theory

Definition of short fibers

Long and slender fibers (L/d>>1) require a very small volume fraction to make a dilute suspension. It is possible to prove that when $V_f < (L/d)^2$, the distance between a fiber and its nearest neighbors is greater than L [3]. No commercially important composites fall into this dilute character.

If the volume fraction of fibers is inside the range $(d/L)^2 < V_f < (d/L)$, then the suspension is said to be semi-concentrated. In this case, the spacing between fibers is smaller than L but larger than d, and interactions between fibers are frequent.

A highly concentrated solution is defined when $V_f > (d/L)$ and the spacing of the fibers is of the order of d.

Tensors of fiber orientation

Tucker *et al*. [5, 9] suggested the use of second-order tensors of fiber orientation as comprehensive descriptors of the state of fiber orientation. The tensors have direct applications to predict both rheological and mechanical properties of fiber suspensions. Moreover, the tensors offer the possibility to represent the statistical distribution of fiber orientation, and may be attributed a physical meaning.

The sum of the diagonal terms of the tensor is the unit, and each of the diagonal values is allowed to vary between 0 and 1. The value of each of the diagonal values stands for the relative orientation around one of the co-ordinate axis. The axis are defined as 1-radial, 2-tangential and 3-thickness directions.

As a result of symmetry, three out-of-diagonal elements only need to be computed. Therefore, five calculations are required to define the second-order tensor, without any simplifying assumptions. Moreover, it is possible to use second- or fourth-order tensors to represent the statistical distribution of fiber orientation. The second-order tensor represents adequately quasi-random fiber orientation states, whereas highly aligned states require the use of fourth-order tensors.

Modeling of fiber orientation

When the composites correspond to the concentrated or semi-concentrated types, it is important to determine the effect of interactions between neighboring fibers upon the fiber orientation. Folgar *et al*. [2] proposed the use of an empirically determined interaction coefficient, C_I. This coefficient depends only on the fiber aspect ratio, L/d, and on the volume fraction, and it is therefore an intrinsic property of the suspension.

However, without a detailed model for describing the interactions between fibers, there is no way to predict C_I, which must be determined experimentally. An empirical expression was suggested by Tucker and Advani [3] to be used whenever an experimentally determined interaction coefficient is not available:

$$C_I = 0.0184 \exp\left(-0.7148\ V_f \frac{L}{d}\right) \qquad (1)$$

which is valid in the concentrated regime ($V_f . L/d > 1$).

From tensors of fiber orientation to properties

An elasticity tensor (T) must verify the following symmetries:

$$T_{ijkl} = T_{jikl} = T_{ijlk} = T_{klij} \qquad (2)$$

For this analysis it is assumed the material as transversely isotropic. To verify those conditions the tensor must have the following form [5]:

$$\begin{aligned} < T_{ijkl} > = & B_1(a_{ijkl}) + B_2(a_{ij}\delta_{kl} + a_{kl}\delta_{ij}) + \\ & B_3(a_{ik}\delta_{jl} + a_{il}\delta_{jk} + a_{jl}\delta_{ik} + a_{jk}\delta_{il}) + \\ & B_4(\delta_{ij}\delta_{kl}) + B_5(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \end{aligned} \qquad (3)$$

The δ_{ij} is the Kronecker delta, similar to the identity matrix (δ_{ij}=1 if i=j, δ_{ij} =0 if $i \neq j$). The $B_1,\ldots,B_5$ are scalar constants, related to the five independent components of a transversely isotropic elasticity tensor.

From the properties of a composite whose fibers lie uniaxially aligned (calculated using the Halpin-Tsai equation) it is possible to determine those scalar constants. The tensor of fiber orientation corresponding to this particular arrangement of the fibers is know (a_{1111}=1 and a_{11}=1, and the other components of the second- and fourth-order tensors are zero).

The fourth order orientation tensor is required to solve Eq. 3. However, the modeling tools allow only the prediction of the second-order orientation tensor components. Tucker *et al.* [5] proposed the use of various closure approximations when the fourth order orientation tensor needs to be calculated from the second order orientation tensor. In this case, an hybrid closure approximation is used instead.

If the orientation averaging procedure is made in terms of stiffness, a constant strain is assumed and a lower bound of the properties is obtained. This was the case hereby considered.

The orientation averaging procedure, includes:

1. Determination of the tensor of fiber orientation.
2. Calculation of the fourth-order orientation tensor using a hybrid closure approximation (the fourth-order tensor can be calculated directly from experimental raw data, if available).
3. Determination of the scalar constants $B_1,\ldots, B_5$ in Eq. 3.
4. Determination of the elements of the stiffness tensor (assuming a constant strain) of the uniaxially aligned composite from Eq. 3.
5. Inversion of the stiffness tensor to obtain the compliance tensor.
6. Rewriting of the compliance tensor into contracted index notation [see *e.g.* 10].
7. Obtaining the principal direction elastic properties (E_{11}, E_{22}, η_{12}, G_{12}, G_{23}) directly from the elements of the contracted index notation compliance matrix.

Modeling of flexure tests

The flexure test was modeled using the FEM Algor software (Algor Inc, USA). The moldings were considered as being made of 10 layers and three materials (Figure 1). The thickness of each layer is dependent on the fiber orientation data obtained in the fiber orientation simulations. For the property definition, each layer was considered orthotropic with respect to the radial and tangential directions. The number of layers used was the same as the number of layers used in the fiber orientation simulations (five in half thickness, symmetric).

Equipment and processes

Molding

A circular center sprue-gated disc, 1.5 mm thick and 114 mm in diameter, was chosen to study the radial divergent flow.

A 10 % by weight glass fiber reinforced grade was used (*Lexan 500 R* from GEPlastics). The material is compounded with a release agent and a flame-retardant additive. The choice for this material was meant to minimize the level of interaction between neighboring fibers during flow.

The molding was done in a molding cell based on a Krauss-Maffei 60/210 A machine of 600 kN clamping force.

The molding program (Table 1) was set to study the effect of melt temperature and flow rate on the stiffness of the moldings.

Flexure tests

The test rig for the three point support flexural tests is represented in Figure 2. A LVDT displacement transducer was located inside the support column to measure the disc deflection. This support is screwed to the load cell in compression mode (mounted onto the base of the machine). The loading nose that applies the load in the center of the disc is driven by the machine crosshead.

An Instron 1122 tensile test machine with a 5 kN load cell was used to determine the flexural behavior of the discs.

The tests were made at 1 mm/min crosshead speed up to a maximum displacement of 0.85 mm to minimize the effect of membrane stresses (about half thickness of the specimens).

Results

Fiber orientation predicted from C-Mold

The fiber orientation distributions obtained in the C-Mold/Fiber program (C-MOLD, USA) show the fiber tendency to become radially aligned in the outer layers ($a_{11} > 0.5$). In the core very high degree of alignment is obtained in the tangential direction ($a_{11} < 0.1 \Rightarrow a_{22} > 0.9$). This is consistent both with theory and previously published results [*e.g.* 11].

Near to the gate, lower radial fiber alignment is observed for all molding conditions. This may be attributed to the divergent flow developing in the conical sprue.

In the intermediate layers, the fibers tend to get more aligned in the tangential direction.

At the core of the moldings a very high alignment in the tangential direction is always predicted. This is a result of the difficulty of the program to model the behavior of the fibers in this region, which is characterized by very low shear stresses.

High injection rate generates lower degree of alignment in the radial direction. Again, this is predictable since high shear stresses develop at lower injection rate.

The effect of the melt temperature on the pattern of fiber orientation is modest. A slight tendency of the fiber orientation to increase in the radial direction is observed.

Mechanical property prediction

The elastic properties (Figures 5 and 6) obtained after the orientation averaging procedure reproduce the pattern of results obtained for fiber orientation (Figures 3 and 4). The stiffness of most of the layers range between 2.8 GPa and 3.3 GPa. Those values compare well with the stiffness given by the raw material supplier (3.3 GPa).

In the core, where the fibers are highly aligned in the tangential direction, high stiffness (up to 4.4 GPa) is obtained. This value is also consistent with the theoretical stiffness (4.9 GPa) calculated using the Halpin-Tsai equations for a fully aligned composite.

The experimental and modeling flexure results are shown in the Table2. It can be observed that the average deviations between the predictions and the experimental results are quite high (19 % in average). For all the molding conditions the stiffness is under-predicted. This result may be an indication that for the material considered, some morphological parameter with a reinforcing effect must be considered.

Conclusions

The pattern of stiffness distribution obtained from the orientation averaging procedure follows the fiber orientation distribution.

The calculated values for the stiffness of the layers using the orientation averaging procedure are consistent with the manufacturer's quoted value for the nominal stiffness of the material.

The skin of the discs is characterized by high stiffness in the radial direction. The core is thick and with higher stiffness in tangential direction.

It is clear the tendency to obtain better predictions when the flow rate is lower.

The differences obtained between predicted and experimentally assessed flexure behavior of the discs are too high to be useful for design purposes.

Further work identifying *missing* morphological features is needed to produce better predictions.

Acknowledgments

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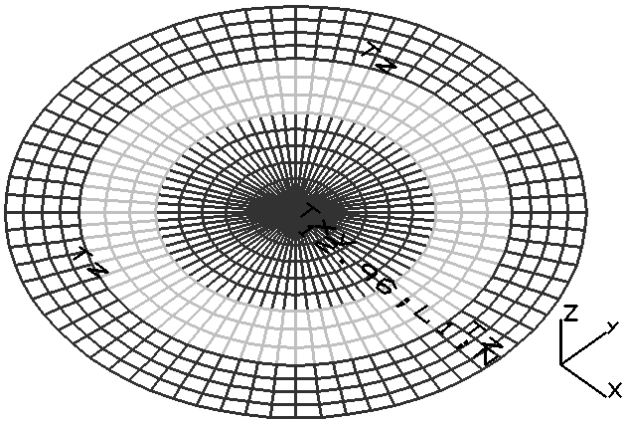

Figure 1. Mesh used in the modeling of flexure tests, three different materials were defined along the flow path

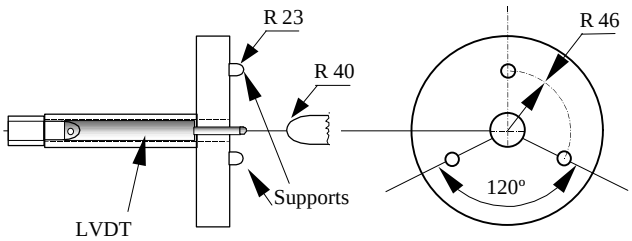

Figure 2. Three-point support rig assembly

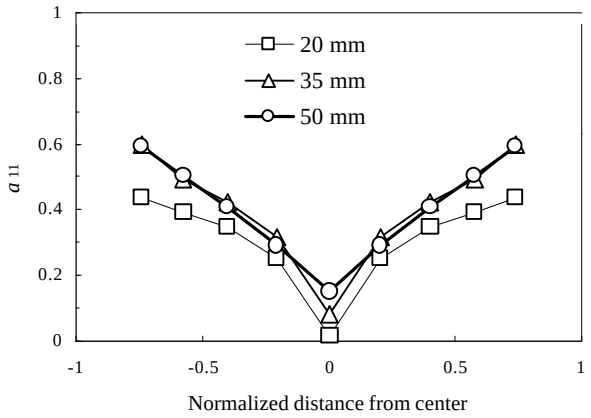

Figure 3. Fiber orientation distribution obtained from C-Mold modeling (320.32)

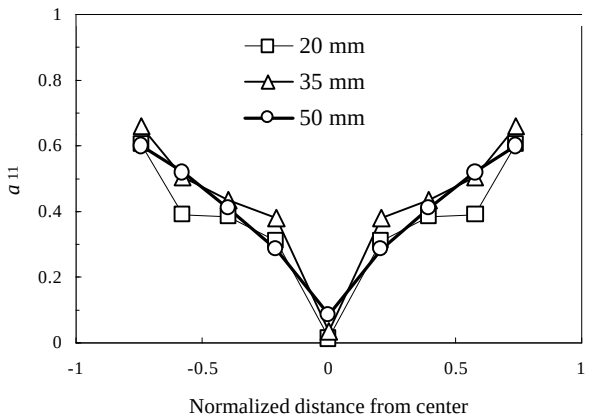

Figure 4. Fiber orientation distribution obtained from C-Mold modeling (320.10)

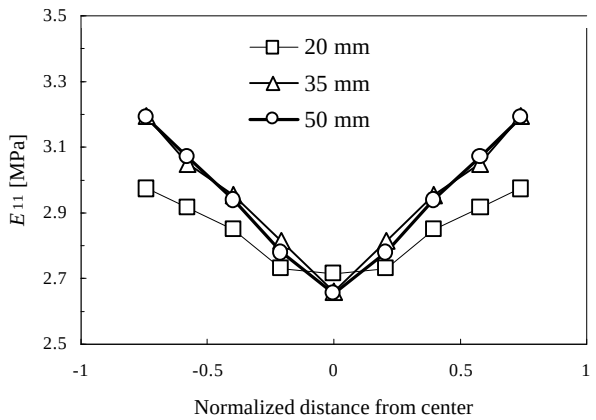

Figure 5. Stiffness in radial direction as calculated with the orientation averaging procedure (320.32)

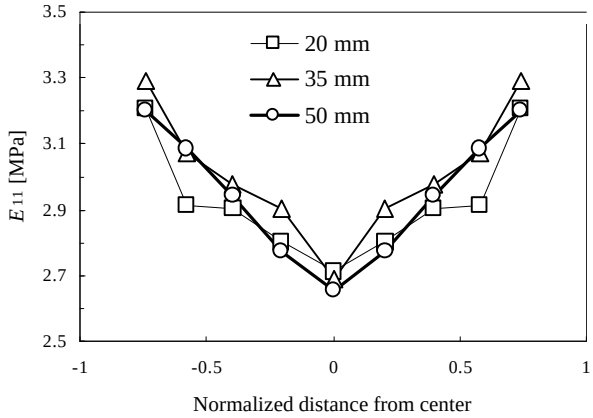

Figure 6. Stiffness in radial direction as calculated with the orientation averaging procedure (320.10)

Table 1 Molding program

Code	Melt temp. (ºC)	Injection flow rate (cm^3/s)	Mould temp. (ºC)
280.10	280	9.7	100
280.14		13.8	
280.32		32.2	
300.14	300	13.8	
320.10	320	9.7	
320.14		13.8	
320.32		32.2	

Table 2. Force/deflection slope in flexural tests and simulations

	Experimental ($kN \cdot m^{-1}$)	FEM prediction C-Mold+Algor	Differences (%)
280.32	12.4 (0.3)	10.1	18.5
280.14	11.5 (0.4)	10.4	9.6
280.10	10.9 (0.4)	10.4	4.6
300.14	14.0 (0.5)	11.0	21.4
320.32	18.6 (0.5)	11.5	38.2
320.14	14.0 (0.2)	10.8	22.9
320.10	15.3 (0.2)	12.5	18.3