A DIRECT PARTICLE LEVEL SIMULATION COUPLED WITH THE FOLGAR-TUCKER RSC MODEL TO PREDICT FIBER ORIENTATION IN INJECTION MOLDING OF LONG GLASS FIBER REINFORCED THERMOPLASTICS

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Abstract

The Polymer Engineering Center at the University of Wisconsin-Madison has developed a particle level simulation model to predict fiber motion at industry relevant fiber concentrations. The model provides a solution to study fiber alignment for long and short fiber-reinforced thermoplastics at the particle level by accounting for all relevant effects, including fiber-fiber interactions. This simulation couples with the Reduced Strain Closure (RSC) Folgar-Tucker model to describe the orientation evolution and interaction coefficients for fibers placed in a simple shear flow. In this work, the process is outlined and the results are compared to existing models for predicting interaction coefficients. Results are then compared to those obtained through injection molding experiments of long glass fiber reinforced polypropylene. A new relationship between fiber aspect ratio and volume fraction will then be proposed.

Introduction

Discontinuous fiber reinforced polymers have recently gained a great deal of popularity due to their superior mechanical properties and lightweight nature. That being said, the final orientation and distribution of the fibers is of utmost importance in the molded part, as these can have important effects on performance of the part. This makes it crucial to be able to predict the fiber flow and final orientation when simulating the molding of discontinuous fiber reinforced parts.

Mold filling software uses models, including the RSC model, for predicting fiber orientation in finished parts. The RSC model relies on two parameters including \( C_1 \), which describes the steady state orientation of the fibers, and \( \kappa \), which describes the total deformation at which the suspension reaches steady state orientation \([4]\). \( C_1 \) and \( \kappa \) rely on the fiber volume percentage and the aspect ratio. As of now, there is not a good model for predicting these values, or even an agreement on the qualitative trend of these values with changing volume fraction and aspect ratio. Software often uses a base value that does not take into account fiber volume percentage and fiber dimensions.

The work described in this paper aims to determine an accurate method for predicting these parameters. These parameters can be determined by using Couette devices or other experimental means as was done by Folgar and Tucker \([1]\). Experimental methods are time consuming and costly, deterring most from taking the time to perform them. A more efficient and less costly means of determining interaction coefficients would allow for more accurate mold filling simulations and improve the quality of parts reinforced with discontinuous fibers.

In this work, a particle level simulation approach based on a mechanistic model is applied to determine the interaction coefficients for the Folgar-Tucker RSC model. The workflow of the presented research work is summarized in Figure 1. The particle level simulation emulates the fiber motion in simple shear flow. Subsequently, the orientation data is used to fit the model parameters of the Folgar-Tucker RSC model. These model parameters are then used to predict the fiber orientation distribution for a large injection molded plaque using Moldex3D (CoreTech System Co., Ltd., Taiwan). Finally, the Moldex3D predictions are compared to actual fiber orientation measurements obtained from micro-computed tomography (μCT) scans.

![Figure 1. Workflow of presented research.](image)

Mechanistic Model

The mechanistic model is a particle level simulation, which models fibers as a collection of nodes that are a fixed length from one another. The segments experience hydrodynamic effects, fiber-fiber interaction, excluded...
volume effects and elastic deformation. The excluded volume force stops fibers from overlapping and is used to model inter-fiber interaction. Discretizing the fibers into more than two nodes or one beam allows fiber bending to occur. The model has not yet implemented fiber breakage.

Figure 2. Forces applied to fibers in mechanistic model [5].

When creating bundles of appreciable volume fraction, typically greater than 3%, there is not a means for generating a random bundle. This necessitates precompression to generate dense fiber suspensions. The precompression software uses the same model, but instead of a shear flow, a compression flow is applied. This allows for the creation of dense bundles by compressing initially dilute suspensions. These bundles do not have a truly random initial orientation, but the RSC model does not depend on initial orientation, so this should not affect final results. There does appear to be a limitation on the maximum density of bundles containing fibers with beam elements of high aspect ratio, but further investigation is necessary.

Figure 3. Fiber bundle before and after compression from 2.5% by volume to 25% by volume [5].

Once an initial bundle of the desired density is obtained, shear flow is applied. The user is able to specify the shear rate, matrix and fiber properties, time step, and simulation time. The time step should be as large as possible to decrease computational time, but if it is too large, it is not possible to produce usable results. Interaction coefficients describe the steady state orientation and the time it takes to achieve, which makes it unnecessary to simulate after the suspension reaches steady state. Physical properties used should correspond to the suspension and processing conditions of interest.

RSC Model

Folgar and Tucker [1] proposed a model that describes the steady state orientation of a fiber suspension in which interaction amongst fibers cannot be ignored. They hypothesized that fiber-fiber interaction tended to randomize the orientation distribution, and proposed the dimensionless parameter \( C_I \) which described this interaction. A high \( C_I \) corresponds to higher fiber interaction, and in turn, lower alignment. The equation in 2D is as follows:

\[
\frac{D\psi}{Dt} = -\frac{\partial}{\partial \phi} \left( \psi \left\{ -\sin\phi\cos\phi \frac{\partial v_x}{\partial x} - \sin^2\phi \frac{\partial v_y}{\partial y} + \\
\cos^2\phi \frac{\partial v_x}{\partial x} \sin\phi \cos\phi \frac{\partial v_y}{\partial y} \right\} \right) + C_I \dot{\gamma} \frac{\partial^2 \psi}{\partial \phi^2}
\]

\( \Psi(\phi) \) describes the orientation distribution, \( v_i \) the velocity and \( \phi \) the fiber angle. This model assumes rigid fibers, negligible inertial and buoyant forces, Brownian motion is negligible and the suspension is incompressible.

Advani and Tucker [2] then added tensor notation in an effort to decrease the number of data points necessary to describe the suspension orientation. These are described as follows:

\[
a_{ij} = \int p_i p_j \psi(p) dp
\]

Where \( p_i \) is a unit vector in the \( i \) direction, and \( \psi(p) \) is the normalized orientation. They then updated the Folgar-Tucker model as follows:

\[
\frac{D a_{ij}}{Dt} = -\frac{1}{2} \left( \omega_{ij} a_{kk} - a_{ik} \omega_{kj} \right) \\
- \frac{1}{2} \left( \gamma_{ik} a_{kj} - a_{ik} \gamma_{kj} - 2 \dot{\gamma}_{kl} a_{ijkl} \right) \\
+ 2C_I \dot{\gamma} (\delta_{ij} - \alpha a_{ij})
\]

where \( \omega_{ij} \) is the vorticity tensor, \( \gamma_{ij} \) is the rate of strain tensor, \( \gamma \) is the shear rate, \( \alpha \) is the number of dimensions, and \( a_{ijkl} \) is the fourth order tensor that is often approximated by the second order tensor using closure approximations.

In the simulations discussed below the orthotropic fitted closure approximation was used [2].
Figure 4. Effect of $C_I$ on steady state orientation.

Wang et al. [4] further modified the Folgar Tucker model. The constant $\kappa$ was added to account for the fact that experimental results showed that the fiber suspensions approached the steady state orientation less quickly than predicted by the Folgar-Tucker Model. This is described as follows:

$$\frac{D\alpha_{ij}}{Dt} = -\frac{1}{2} (\omega_{ik}a_{kj} - a_{ik}\omega_{kj}) + \frac{1}{2}\lambda(\gamma_{ik}a_{kj} - a_{ik}\gamma_{kj})$$

$$-2[a_{ijkl} + (1 - \kappa)(L_{ijkl} - M_{ijmn}a_{mnkl})]\gamma_{kl}$$

$$+ 2\kappa C_I\gamma(\delta_{ij} - \alpha a_{ij})$$

If $\kappa = 1$, the model returns to that of Advani and Tucker, thus a lower value of $\kappa$ corresponds to a slower orientation evolution. This is the model that was used to describe the orientation of the shear cell simulations in this work.

Figure 5. Effect of $\kappa$ on the rate at which steady state orientation develops.

Injection Molding Experiments and Simulations

For the experimental part of this work, center-gated plaques were molded at two different fiber concentrations. The material used in this study is a commercially available glass fiber-reinforced polypropylene (PP) at 20% wt. and 40% wt. fiber concentration (SABIC®, STAMAX 20YM240 and 40YM240). Table 1 summarizes the material properties of interest.

<table>
<thead>
<tr>
<th>Material Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nominal Fiber Density [%wt]</td>
<td>20 and 40</td>
</tr>
<tr>
<td>Nominal Fiber Density [%vol]</td>
<td>8.2 and 19.1</td>
</tr>
<tr>
<td>Initial Fiber Length [mm]</td>
<td>15</td>
</tr>
<tr>
<td>Fiber Diameter [µm]</td>
<td>19 ±1</td>
</tr>
<tr>
<td>Density Fibers [g/cm³]</td>
<td>2.55</td>
</tr>
<tr>
<td>Density PP [g/cm³]</td>
<td>0.905</td>
</tr>
</tbody>
</table>

The material was processed on a 1,600-ton KraussMaffei injection-molding machine (KM 1,600/12,000/4,300 MX L) at the Fraunhofer Project Centre for Composites Research at Western University, Canada. The processing settings follow the official processing guidelines by SABIC® and are summarized in Table 2.

<table>
<thead>
<tr>
<th>Molding Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Melt Temperature [°C]</td>
<td>260</td>
</tr>
<tr>
<td>Mold Temperature [°C]</td>
<td>60</td>
</tr>
<tr>
<td>Injection speed [cm³/s]</td>
<td>400</td>
</tr>
<tr>
<td>Back Pressure [bar]</td>
<td>5</td>
</tr>
<tr>
<td>Holding Pressure [bar]</td>
<td>400</td>
</tr>
<tr>
<td>Holding Time [s]</td>
<td>25</td>
</tr>
</tbody>
</table>

A square center-gated plaque was molded, which is illustrated in Figure 6. The plaque has an edge length of 610 mm and a thickness of 2.4 mm. The local fiber orientation of the injection-molded plaques was measured using μCT at the location indicated in Figure 6. Furthermore, the fiber length was measured in the purged material to determine the average fiber aspect ratio in the material before the material is injected in the mold. For the 20 % wt. concentration, the fiber length was measured to be 4.7 mm (aspect ratio of 250) and 2.7 mm (aspect ratio of 140) for the 40 % wt. concentration material.

The injection molding experiments were simulated using Moldex3D. The fiber orientation was predicted using the implemented Folgar-Tucker RSC model using the
model parameters found with the mechanistic model predictions. Ultimately, the predicted and measured fiber orientation were compared to evaluate the performance of the optimized Folgar-Tucker RSC parameters.

![Illustration of the molded plaque and the location for the fiber orientation measurement.](image)

**Mechanistic Model Simulations**

The physical properties of the fibers and matrix that were used in simulation can be seen in Table 3 and Table 4 below.

Table 3. Constant values in simulations.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Viscosity (Matrix) [Pa s]</td>
<td>84.3</td>
</tr>
<tr>
<td>Fiber Young’s Modulus [GPa]</td>
<td>73</td>
</tr>
<tr>
<td>Fiber Strength [MPa]</td>
<td>2600</td>
</tr>
<tr>
<td>Shear Rate [s⁻¹]</td>
<td>150</td>
</tr>
</tbody>
</table>

Table 4. Values varied in simulations.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Weight Fraction [%]</td>
<td>5, 10, 20, 30, and 40</td>
</tr>
<tr>
<td>Volume Fraction (VF) [%]</td>
<td>1.8, 3.8, 8.2, 13.2, and 19.1</td>
</tr>
<tr>
<td>Aspect Ratio (L/D) [-]</td>
<td>25, 50, 100, 150, and 200</td>
</tr>
</tbody>
</table>

The bundles were of equal size proportional to fiber length (L) at 1.2L x 1.2L x 0.75L. The x-y plane is sheared, which is why the z length was smaller than the fiber length itself. It was chosen to be smaller to save computational cost. The very low aspect ratio and fiber concentrations did warrant a slightly larger cell due to the small number of fibers they contained at the aforementioned dimensions.

Bundles ranged from 60 to 10,500 fibers. All fibers were made up of 5 segments in an effort to minimize computational expense. Once bundles were generated, they were sheared for 1 second using a step size of 10⁻⁶ seconds. This was the largest step size that generated good results. The strain for each simulation was at least 150 to ensure that a steady state orientation was reached. Subsequently, the model parameters, C₁ and κ, were fitted to the results of the mechanistic model simulations. A genetic algorithm was used to fit the model to the data set. One set of results of the optimization procedure is shown in Figure 7 (10% wt., L/D = 100).

![Evolution of a₁₁ tensor component in shear flow.](image)

Transient effects were observed in a number of cases, which necessitated running those simulations for additional time. The longest any simulation was run was 2 seconds, or twice the baseline time.

The data obtained from the mechanistic model showed that C₁ tended to increase with an increase in the product of volume fraction and aspect ratio (VF*(L/D)). In Figure 8, the C₁ values are plotted by aspect ratio. The best-fit linear trend lines had R² values ranging from 0.51 to 0.85.

![Interaction Coefficients determined by mechanistic model.](image)
As one can see, the interaction increased as $VF^*(L/D)$ increases. It also appears that higher aspect ratios led to lower $C_I$ values. After the data was fitted, the slopes were taken and plotted vs. aspect ratio in an attempt to find a trend. This can be seen in Figure 9 below.

![Figure 9. Slope of $C_I$ curve plotted as a function of aspect ratio.](image)

These two plots suggest there is a linear relation between $VF^*(L/D)$ and $C_I$ and the slope is a function of the negative exponential of the aspect ratio. With this data, the best fit is described as:

$$C_I = 0.7201 \times \left(\frac{L}{D}\right)^{-1.228} \times (VF * (\frac{L}{D}))$$

This suggests that aspect ratio may have an effect that is separate from the effect caused by the combination of aspect ratio and volume fraction.

The mechanistic model’s trends agree with the experimental data of Folgar and Tucker [1], who also showed an increase in the interaction coefficient with an increase in $VF^*(L/D)$. This appeals to intuition, as with more and longer fibers, it makes sense that they would be more likely to interact with one another. Bay [3] on the other hand, proposed quite the opposite. From his own experiments, he proposed that $C_I$ decreased with $VF^*(L/D)$ as shown in Figure 10.

![Figure 10. Comparison of the findings of Bay and Folgar [3] where cL/d is the product of volume fraction and aspect ratio. The squares are Folgar and Tucker’s data points.](image)

Results from the mechanistic model suggest that it is a function of not the product of aspect ratio and volume fraction, but of each individually. This makes it difficult to compare to Bay or Folgar and Tucker, but the general trend agrees with Folgar and Tucker in that interactions tend to increase with an increase in $VF^*(L/D)$. Figure 11 shows a comparison between the results of Bay, Folgar and Tucker, and the mechanistic model for an aspect ratio of 150.

![Figure 11. Comparison of mechanistic model results to experimental results](image)

**Comparison to Injection Molded Plates**

The proposed optimization scheme to determine the Folgar-Tucker RSC model parameters was further tested for injection molded plaques. The injection molding process was simulated in Moldex3D and the fiber
orientation was estimated with the implemented Folgar-Tucker RSC model. The optimized parameters obtained from the mechanistic model simulation for the 20\%wt. and 40\%wt. material are summarized in Table 5.

Table 5. Folgar-Tucker RSC parameters used for Moldex3D simulation.

<table>
<thead>
<tr>
<th>Fiber Weight Concentration</th>
<th>Fiber Aspect Ratio</th>
<th>Optimized ( C_1 )</th>
<th>Optimized ( \kappa )</th>
</tr>
</thead>
<tbody>
<tr>
<td>20%wt.</td>
<td>250</td>
<td>0.022</td>
<td>0.411</td>
</tr>
<tr>
<td>40%wt.</td>
<td>140</td>
<td>0.027</td>
<td>0.304</td>
</tr>
</tbody>
</table>

The predicted fiber orientation results and the measurements are compared in Figure 12 and Figure 13 for the 20\%wt. and 40\%wt. trials, respectively. Generally speaking, the predicted fiber orientation shows good agreement with the experimental results. The average orientation in flow direction \( (a_{11}) \) in the shell layers are within ±0.05 of the measured data. However, there is a bigger discrepancy between measurements and predictions in the core layer of the part. The measurements suggest a more distinct cross-flow orientation \( (a_{22}) \) in the center of the part whereas the Folgar-Tucker RSC prediction estimates a much lower cross-flow orientation for both fiber concentrations.

![Figure 12. Comparison of measured fiber orientation and Moldex3D predictions for the 20\%wt. injection molded sample.](image)

![Figure 13. Comparison of measured fiber orientation and Moldex3D predictions for the 40\%wt. injection molded sample.](image)

This discrepancy needs to be further evaluated to identify whether it stems from the optimized \( C_1 \) and \( \kappa \) values, from the Moldex3D simulations or more fundamentally from the Folgar-Tucker RSC model. One aspect that needs to be studied further is the heterogeneous fiber density distribution found in injection molded parts, as discussed in [6]. Fibers tend to agglomerate in the center of injection molded parts with a distinct fiber density distribution through the thickness. Together with the dependency of \( C_1 \) and \( \kappa \) on the fiber concentration, this would suggest the model parameters should not be treated as constant values in injection molding simulations. It might more appropriate to make both parameters depend on the spatial location and the local fiber concentration:

\[
C_i = f(x,y,z,\phi_f)
\]

where \( \phi_f \) is the local fiber volume concentration.

Conclusions and Future Work

The proposed methodology of using a particle level simulation to simulate the fiber suspensions in the concentrated regime proved to be a valuable tool to determine continuum model parameters. The shear cell with periodic boundary conditions allows one to study the motion of fibers and their interaction on a micro level. After running shear simulations using the mechanistic model, it was determined that the interaction between fibers tended to increase as the volume fraction increased as proposed by Folgar and Tucker [1]. An empirical relation was also proposed to describe the behavior of the interaction coefficient.

The mechanistic model was also used to obtain continuum model parameters for the simulation of injection molded parts. The obtained simulation results were compared to fiber orientation measurements. It was found...
that the simulation results show good agreement in the shell layers, but larger discrepancies in the core region.

In the future, the research using the mechanistic model approach will continue to gain a better understanding of the underlying physics of the motion of fibers and their interactions in the concentrated regime. Further sensitivity analyses will be performed to estimate the impact of aspect ratio and fiber concentration on the orientation behavior of fibers in simple shear flow.

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References