PARTICLE LEVEL SIMULATION OF FIBER MOTION TO DETERMINE CONTINUUM BASED MODELS PARAMETERS FOR FIBER ORIENTATION PREDICTION

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Abstract
A particle level simulation was used to simulate fiber suspensions in the concentrated regime. Parameters used in large scale simulations were obtained through this simulations, specifically the Interaction Coefficient C_i of the Folgar-Tucker model. The values obtained are within the range of possible values of the parameter.

1. Introduction

Fibers are used as fillers in the production of plastic components that require to be light weight and strong. Glass fibers and Carbon fibers are the most common types of fibers used to reinforce plastics. The mechanical properties of composite materials is determined by the following characteristics: fiber volume fraction, fiber length distribution and fiber orientation distribution.

Parts will be stronger if fiber length and volume fraction are high, and they will be stronger in the direction of fiber alignment. The complexity of production is proportional to the fiber length therefore for high volume production of parts the use of discontinuous fibers is common. Parts are often produced via injection or compression molding. The fiber orientation in parts produced using these techniques is defined by the flow behavior of the composite mixture. In general, fibers will try to align themselves with the direction of the flow. The direction of the flow during processing depends on many variables; such as geometric characteristics of the cavity, fluid properties and process parameters. In the past decades, continuum based models have been developed, which treat the fibers as a continuum and can be used to estimate their orientation, given that the flow behavior is known.

The most popular model is the so called Folgar-Tucker model[1], which is a rotary diffusion model. It is implemented in most commercial filling simulation packages. It only requires a scalar parameter C_i known as the interaction coefficient, which is unique for each fiber-fluid mixture, and is usually found experimentally. More sophisticated models have been developed such as the Reduced Strain Closure (RSC) model by Wang[2], which adds a parameter κ to slow down the orientation kinetics, κ is also found experimentally. And the Anisotropic Rotary Diffusion (ARD) model by Phelps and Tucker[3], which treats the interaction coefficient as a second order tensor. These models have been extensively

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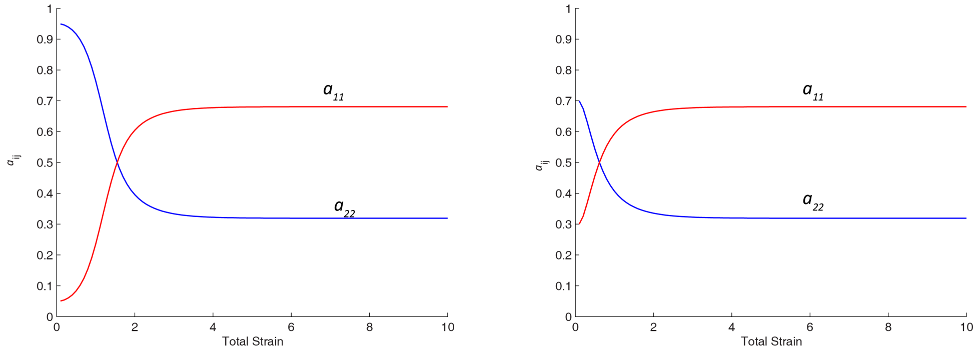

Figure 1: Planar orientation tensor development for different initial orientations and same value of C_i

used in industrial applications and given that the parameters used in the simulation are correct, the results obtained with them are satisfactory.

Although these kinds of models exist, the details of concentrated fiber suspension dynamics are not well understood. Particle level simulations have been used in the past to aid in the understanding of these systems. In these simulations each single particle is accounted for, and approximated as a chain of rigid bodies. Most of the results obtained with these simulations, agree qualitatively and quantitatively with experimental results. Furthermore, they have been used to obtain the parameter C_i for the Folgar-Tucker model with some success[4].

As mentioned earlier the parameters needed to use the continuum based models are obtained experimentally. Parts are molded and orientation is measured in different locations. The parameters are adjusted in a mold filling simulation of the part so the predicted orientation matches the measured orientation. This methodology presents many disadvantages; measuring fiber orientation is expensive and information about the system is just known at the end. Obtaining this parameter numerically has advantages over obtaining it experimentally; in a numerical set up all the parameters can be accurately controlled, detailed information is always available such as fiber content, fiber length distribution and fiber orientation and is relatively inexpensive to perform.

The objective of the current work is to use a particle level simulation to calculate fiber suspension parameters to be used in continuum based models, specifically the interaction coefficient Ci.

2. Dynamics of Concentrated Solutions

Folgar and Tucker[1] proposed a phenomenological model based on Jeffery's equation[5] for a single fiber to describe the motion of fibers in concentrated solutions, with fiber reinforced composites applications in mind. They noticed that in concentrated solutions most fibers were aligned with the flow, just as described by Jefferys equation. However the breadth of the orientation distribution did not match Jeffery's. They reasoned that this deviation was due to fiber interactions. They proposed to add a diffusion term in Jefferys equation to account for this. According to them, interactions tend to randomize the orientation distribution. Particles that interact move from regions of higher orientation to regions of lower orientation, this is analogous to a transport problem where property diffusion is driven by changes in its gradient. Following this idea, there is diffusion of orientation driven by orientation gradients in fiber suspensions. The frequency of fiber interactions is proportional to $\dot{\gamma}$, as the faster the fibers rotate, higher are the chances of fiber collisions. To account for all other factors that might affect the interactions of the fibers such as fiber dimensions, fiber content, etc... they proposed a dimensionless parameter C_i called

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the interaction coefficient. The parameter C_i determines the steady state orientation of a suspension subjected to a constant deformation rate. Low values of C_i represent suspensions were interactions are not important and resemble orientations as determined with Jeffery's model and therefore a highly preferred orientation in the flow direction.A high C_i would yield a significantly lower preferred orientation in the flow direction than Jeffery's equation yields. The steady state orientation is independent of the initial orientation, it only depends on the type of flow and the value of C_i. Following this, the C_i value is only valid if the orientation used to fit it is a steady state orientation. Figure 1 shows how a typical orientation distribution changes with total deformation for different initial orientations calculated with the Folgar-Tucker model and same C_i. The component in the direction of the flow increases and reaches a steady state that is the same for both initial orientation states.

3. Level Particle Model Description

The model that will be used in this work is similar to that proposed by Schmid[6] and later by Lindstroem[7]. Fibers are modeled as a chain of rigid capped cylindrical segments connected by ball and socket joints. In

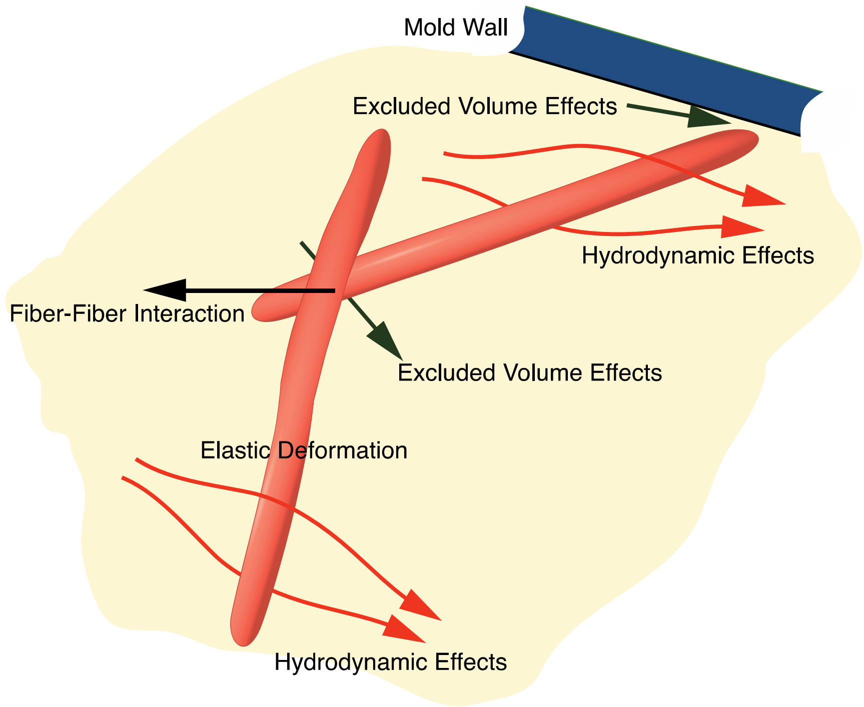

Figure 2: Effects acting on fibers when moving in a suspension

our model, the positions, x_i, velocities v_i and angular velocities ω_i are stored at the ends of the segments i. The fibers are immersed in a viscous fluid that is flowing at a low Reynolds number, therefore inertial effects are neglected. The flow field U^∞ is known. Segment i will experience different forces: Drag forces from the surrounding fluid (F^H), inter-fiber interaction forces with segment j (F^C_{ij}), and intra-fiber forces exerted by adjacent segments (X). The translational equation of motion is written as:

$$0 = F^H + \sum_j F^C_{ij} + X_i - X_{i+1} \tag{1}$$

The rotational equation of motion is analogous but includes an elastic recovery term M^b that includes the Young's Modulus of the fiber and a Hydrodynamic torque T^H:

$$0 = T^H - r_i \times X_{i+1} + \sum_j r_{ij} \times F^C_{ij} + M^b_i - M^b_{i+1} \tag{2}$$

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If a fiber has more than one segment, an extra constrain that enforces connectivity between the different segments is used:

$$v_i + \omega_i \times (x_{i+1} - x_i) - v_{i+1} = 0 \tag{3}$$

where x_i is the position of segment end i, and x_{i+1} is the position of segment end $i + 1$. To compute the hydrodynamic force and torque, the segments are represented as a a succession of beads, the force and torque in a segment is the sum of the force and torque over all beads that form the segment. Equations (Eq. 1), (Eq. 2) and (Eq. 3) constitute a linear system of equations in which the unknowns are the linear velocity v_i and the angular velocity ω_i of segment i. Fibers are advanced in time by integrating the velocities with a Runge-Kutta 4 time stepping.

To represent infinite solutions in a shear rate a cubic cell is used. The cell is filled with as many fibers as required to reach the desired volume content. Due to high fiber aspect ratios the limit in volume fraction that can be reached by randomly generating fibers is around 3%[8]. To overcome this limitation Fibers are randomly generated in a cluster with a low volume fraction, the cluster is then compressed in one direction to increase the fiber volume fraction. A shear flow is imposed onto the fibers. Lees Edwards periodic conditions as described by[9] are used, this takes care of the periodicity in the direction perpendicular to the flow and gets rid of wall effects in the simulations.

The cluster is sheared until a steady state orientation quantified as a tensor is achieved. To obtain the interaction coefficient, a Gauss-Newton fitting is used to adjust the value of C_i to match the orientation in the steady state region. The orientation evolution is computed using the tensorial representation[10] and the hybrid closure approximation[11] for the 4-th order tensor computation.

4. Numerical Results

4.1. Comparison with experimental results

Folgar and Tucker[1] sheared a suspension of polyamide fibers in silicone oil in a couette device. The suspensions were sheared for long periods of time to ensure that a steady state had been reached, and the orientation was measured. Numerical experiments were run with the same properties of the experiments to test the validity of our model. The parameters used in the experiment and in the simulation are listed in table 1. The simulations were run following the procedure described in the previous section; a cluster of

Table 1: Folgar and Tucker's experiment parameters

Property	Value
Fiber Diameter	0.406 mm
Fiber Length	15.6 mm
Aspect Ratio	16
Fiber Young's Modulus	2.62x10^9 Pa
fiber Aspect Ratio	97.5 Pa-s
Oil Viscosity	97.5 Pa-s
Volume Fraction	1%, 8% and 16%

fibers with the desired fiber content was generated and then sheared until a steady state in the orientation tensor components was achieved. All simulations reached a steady state where the fibers were highly aligned with the flow. The steady state value of the component aligned with the flow(a_{11}) decreased with

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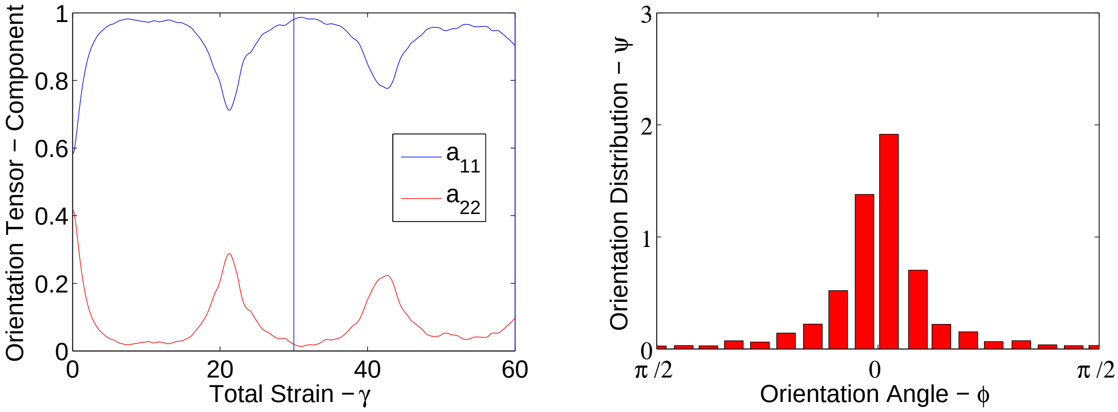
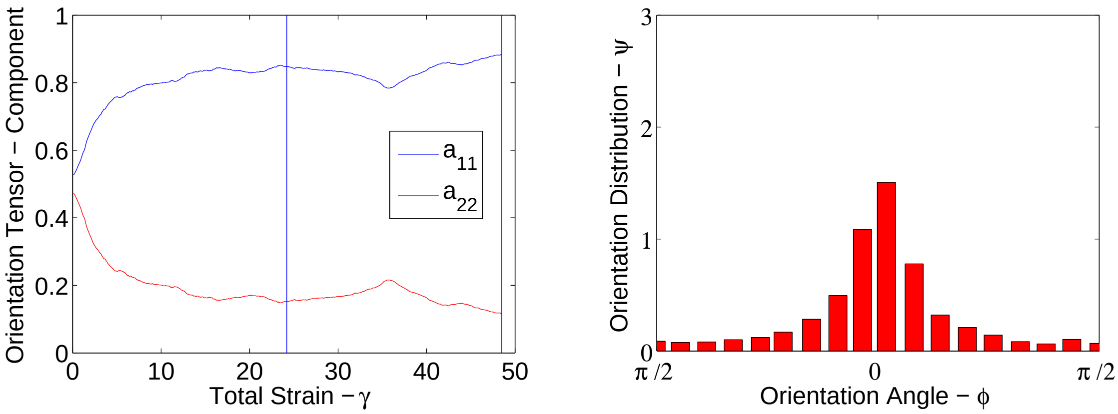
the volume fraction, as the interactions in the system were more significant. The average orientation tensor components in the steady state region were compared with the tensor components obtained with the orientation distribution reported by Folgar and Tucker. Figures 3, 4 and 5 show the results, and the region where the components were averaged. In all cases the value of the computed steady state orientation tensor is within a 3% of the reported value. The results for 1% show oscillation due to the lack of interactions. However the average steady state orientation is close to the reported one. In general the results agree with the experiments.



(a) Evolution of a_{ij} computed numerically, Average a_{11}=0.92 a_{22}=0.08

(b) Experimental steady state planar orientation[1], a_{11}=0.88 a_{22}=0.12

Figure 3: Results for 1% fiber content



(a) Evolution of a_{ij} computed numerically, Average a_{11}=0.84 a_{22}=0.16

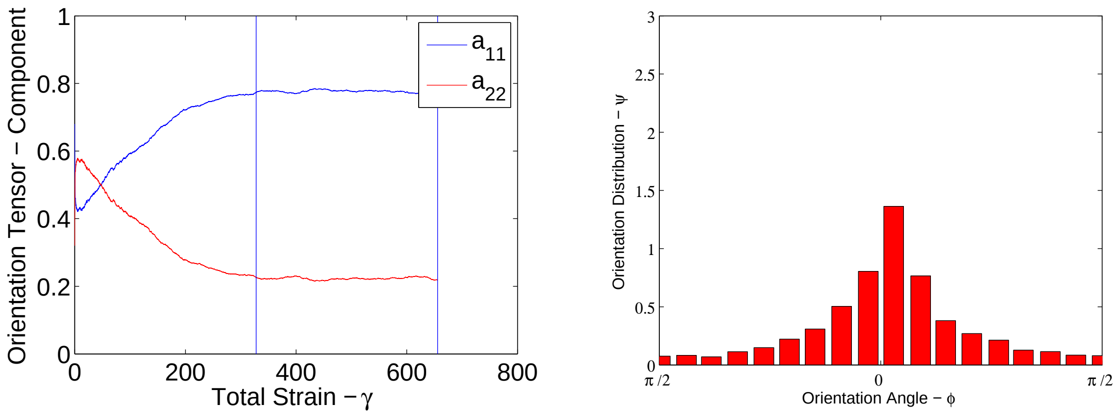
(b) Experimental steady state planar orientation[1], a_{11}=0.81 a_{22}=0.19

Figure 4: Results for 1% fiber content

4.2. Industrial grade system

Properties of an industrial grade system were used to estimate values of C_i. The material used was Sabic's STAMAX®. The fiber length used was the fiber length measured in injection molded plaques with the same material. The viscosity used was that of the unfilled matrix and provided by the supplier. The weight fraction of the the material is 30% which is 13% by volume. Table 2 lists the values used in the simulations. Simulations were run following the same procedure describe in the previous sections.

We present the history of the tensor components of one of this simulations in Figure 6. The components



(a) Evolution of a_{ij} computed numerically, Average a_{11}=0.77 a_{22}=0.23

(b) Experimental steady state planar orientation[1], a_{11}=0.77 a_{22}=0.23

Figure 5: Results for 1% fiber content

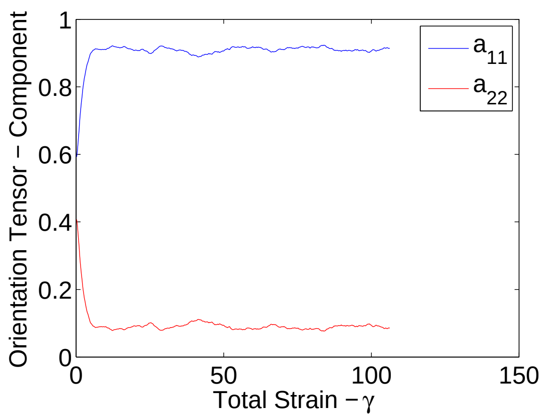


Figure 6: Orientation tensor components for an industrial grade material

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Table 2: Industrial grade material parameters

Property	Value
Fiber Diameter	0.406 mm
Fiber Length	15.6 mm
Fiber Young's Modulus	2.62x10^9 Pa
Fiber Aspect Ratio	97.5 Pa-s
Matrix Viscosity	97.5 Pa-s
Volume Fraction	13%

reach a steady state orientation. The interaction coefficient obtained for this material was 0.014, which is within the range reported in literature[12].

5. Conclusion

A particle level simulation has been used to estimate the interaction coefficient of the Folgar-Tucker model. The model was validated with reported experiments by Folgar and Tucker. Simulations were run with an industrial grade material and interaction coefficients were estimated. The values are within the range reported in the literature. Further validation of the industrial grade material has to be done with injection molded parts.

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