# COMPUTER PREDICTION OF THE BEHAVIOR OF FIBER-REINFORCED COMPOSITES DURING MOLDING

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## Abstract

Mechanistic Computer simulations of flexible fiber suspensions are developed to study the molding of fiber reinforced composites. Fibers are modeled as chains or rigid beads connected by springs. Parameters such as fiber concentration fiber length and stiffness can be modified to match specific processing conditions. Simulation results include final fiber orientations and fiber distributions within a molded part. Specific applications for this type of simulations are compression molding of Sheet Molding Compound, where defects such as Fiber-Jamming and Fiber-Matrix separations are difficult to predict and still not well understood.

## Background

Manufacturing processes involving polymers are characterized by the influence played by processing conditions in final part properties. When a polymeric part is processed, whether it is molded, extruded or injected, not only the geometry but also mechanical, electrical as well as many other physical properties are also determined [1]. Variations in parameters such as mold velocity, injection pressure or mold temperature will lead to parts with substantially different characteristics.

Perhaps in no other application is this behavior more evident as it is in the case of fiber reinforced composites. When a polymer composite is molded, fiber orientation within the part will change as the flow evolves, and the mechanical properties of the part will depend on the fiber distribution at the moment the flow freezes [2]. Additionally, a set of molding parameters or variations in part geometry can lead to uneven fiber distributions to the extent that Fiber-Matrix separation may take place. This effect is also known as Fiber Jamming and is characterized by the formation of bundles of interlocked fibers that interfere with the free flow of fibers [3] leading to zones void of fibers. To be able to predict this type of defects a model that includes fiber flexibility is required.

Currently, the onset of such defects is controlled with trial an error techniques. However these techniques are economically unsound plus the amount of defective parts remains a concern. This situation translates into added production costs which can be minimized with the development of the proper computational tools. Our research is focused on developing techniques that lead to the prediction and prevention of Fiber-Matrix separation and Fiber-Jamming.

Most of the existing work in the area of fiber matrix separation and defect characterization is experimental [4,5,6]. From this work it is known that molding setups with higher mold velocities and low resin viscosities are more prone to cause uneven fiber density distributions [7]. Theoretical studies have been conducted to determine the viscosity of Sheet Molding Compounds (SMC) and the constitutive equations governing the flow [8,9]. Computer simulations of fiber suspensions are also part of ongoing research in the paper-making industry, where special interest is given to the prediction of flock formation [10,11].

This work starts by presenting a computer algorithm that models fiber flow in a fluid matrix. Special emphasis is placed in the inclusion of fiber flexibility in the model. Following sections present results obtained with this algorithm for different fiber setups.

## Computer Algorithm

The main idea behind the algorithm presented in this section is to model fibers as chains of connected rigid beads. Figure 1 shows a cartoon of a fiber and its equivalent bead and spring representation. In this model beads are connected with each other by springs. The flexibility of the springs can be adapted to simulate different fiber stiffness. Parameters such as number of beads per fiber and distance between beads are input parameters that can be modified to simulate different conditions.

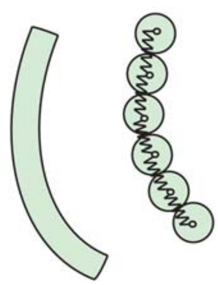

Figure 1: Original fiber and its equivalent bead and spring fiber.

The force balance for a single bead is given by:

$$f_{ij}^{d} + f_{ij}^{f} + f_{ij}^{xv} + f_{ij}^{c} + f_{ij}^{b} = 0 \qquad (1)$$

The term $f^d$ is the hydrodynamic drag force on a bead. This force is caused by the interaction between the bead and the liquid and is given by:

$$f_{ij}^{d} = -\varsigma_f (v_{ij} - u_{ij}) \qquad (2)$$

where $\varsigma_f$ is the friction coefficient, $v_{ij}$ is the velocity of the bead and $u_{ij}$ is the velocity of the flow. The force $f^f$ is the friction force between beads. This friction can be Coulombic, *i.e.* the product of a normal force and a friction coefficient, but can also include a lubrication-type force. The force $f^{xv}$ is the excluded volume between beads and is used to avoid particle overlap when particles move too close to each other. The force $f^c$ is the connector force between neighboring beads. Since beads are connected by springs, the connector force is given by the reaction forces that arise as the springs are deformed. Finally $f^b$ is the fiber bending force and works similarly to a spring force: as the fiber is bent a reaction force proportional to the deformation starts to develop.

The velocity of the bead can be defined as:

$$v_{ij} = \frac{dx_{ij}}{dt} \tag{3}$$

Combining this equation with the equation of motion and defining the drag force in terms of the velocities, an expression for the change of position with respect to time is obtained:

$$\frac{dx_{ij}}{dt} = u_{ij} + \frac{1}{\varsigma_f}(f_{ij}^{f} + f_{ij}^{xv} + f_{ij}^{c} + f_{ij}^{b}) = 0 \tag{4}$$

All forces in the right hand side of the equation are functions of the bead positions and can be computed for a given time step. The only remaining unknown is the velocity of the fiber beads. In a typical simulation eq. 4 is solved for each fiber bead at each time step. This equation is integrated in time to find the new position of each segment and therefore all fibers in the suspension.

# Results

## Fiber flexibility

As it was mentioned before, one of the main objectives of this algorithm is to have the capability to model fiber flexibility. Figure 2 shows the superposed simulation results obtained for a rigid and a flexible fiber under shear flow. In this type of flow the upper and lower walls of the box move in opposite directions. In order to model stiff fibers, high bending forces between beads $f^b$ are used while flexible fibers are modeled with low bending forces. From this figure it is observed that the rigid fiber rotates but does not translate. This behavior is in accordance with both theoretical and experimental results [2]. In the other hand, the flexible fiber rotates and translates but also changes shape. This comparison illustrates how fiber flexibility has a direct influence in fiber position. In a simulation at high fiber concentrations, where there is increased contact between fibers, this effect will have a dominant role.

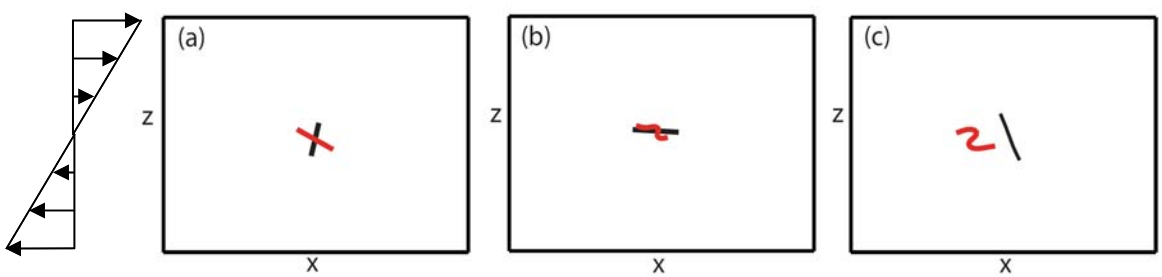


Figure 2: Flexible Vs. Rigid fiber at increasing time steps (From (a) to (c)).

## Fiber Orientation

Computer simulations were performed for fiber suspensions under one dimensional extensional flow. This type of flow can be used to model the flow of an SMC charge and is governed by the equations:

$$v_x = \frac{\dot{h}}{h}x \tag{5}$$

$$v_z = \frac{-\dot{h}}{h} z \tag{6}$$

where $h$ is the mold thickness and $\dot{h}$ is the mold closing velocity. In these equations the volume reduction in the (z) direction is compensated by a volume increase in the (x) direction, bearing resemblance to the way a polymer charge is compressed.

Experiments where conducted in order to study the influence of initial mold coverage in final fiber distribution. A set of 400 fiber each of them with 20 beads where randomly positioned in a virtual rectangular mold. The volumetric fiber content for all simulations was of 1.7% and a fiber length to diameter aspect ratio $r_p$=L/D of 60 was used. Figure 3 shows the initial fiber distribution for a charge covering 33% of the mold. The charge was initially positioned on the left corner of the mold and the flow was in the positive (x) direction. Simulations ran until the mold was completely filled. Similar experiments where also conducted for 50 and 66 % mold coverage. In order to compare the results with existing fiber orientation prediction models, fibers where kept rigid in these particular simulations.

Using the final fiber positions obtained from the simulations, fiber orientation was calculated for all three cases. Figure 4 shows the fiber orientation distribution for the three simulations. The bars in the figure are the simulation results, while the continuous line is the predicted orientation obtained with the Folgar-Tucker model using an interaction constant $C_I$=0.15.

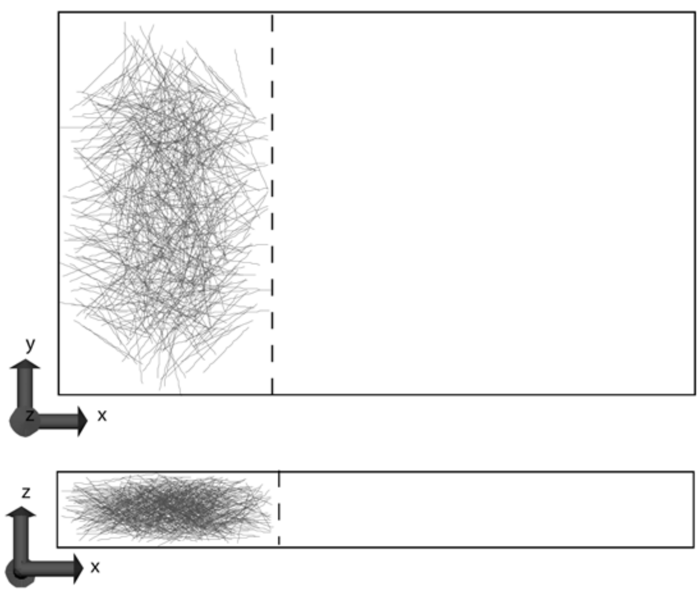


Figure 3: Initial fiber distribution 33% mold coverage (Top and side view).

It is observed that simulations correlate well with the predicted values. It is however noticed that at higher mold coverage results start to differ from predicted values. Fibers in the simulations take more time to orient than it is predicted. This behavior is attributed to fiber interlocking and collisions. At the start of the flow fibers try to orient with it, but they will collide with other fibers and tend to entangle. As fibers become more oriented, collisions will decrease and fibers will eventually orient but at a slower pace than predicted.

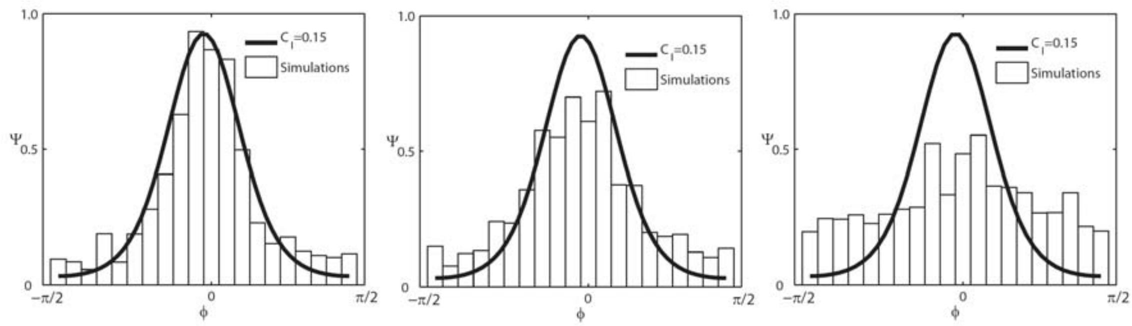


Figure 4: Fiber distribution at 33, 50 and 66% mold coverage (from left to right).

## Simulations of compression molding of SMC

A special algorithm was developed to locate the fibers like they are in a real SMC. This algorithm works by randomly locating fibers in increasing two dimensional layers. The number of fibers per layer as well as the number of layers can be modified.

An added advantage of this configuration is that higher fiber volumetric contents can be reached. With the simulations presented in the previous section it is possible to go as high as 2% volumetric content, a value still far from real molding applications. With the virtual SMC simulations it is possible to run simulations up to 20% volumetric content. Simulations higher than 20% are also possible. However due to the increased amount of fiber interactions, the calculation time would significantly increase.

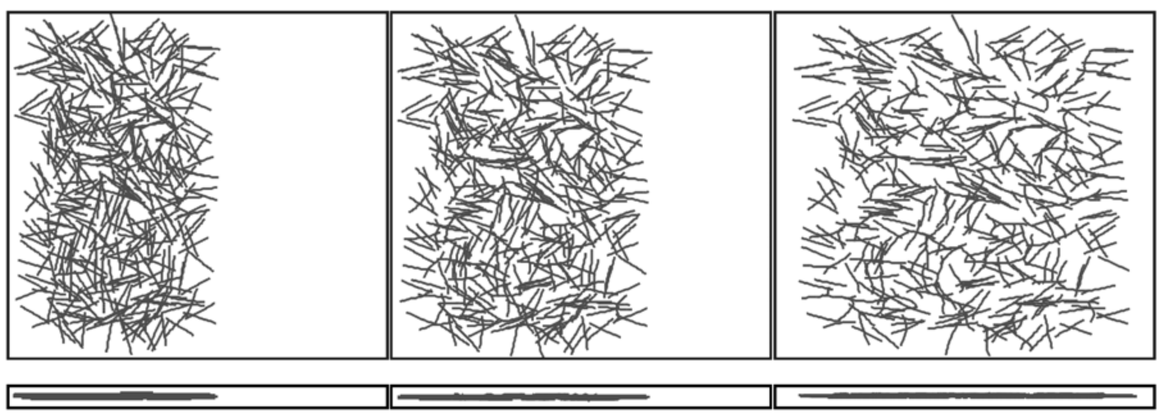

Figure 5: Top and side view of fiber distribution in a virtual SMC at increasing time steps (From left to right).

Figure 5 presents a sequence showing simulation results for the compression molding of a virtual SMC. These results where obtained using 400 fibers each of them with 25 segments and a fiber concentration of 4%. It is observed that the thickness of the charge has decreased by positioning the fibers in a virtual SMC. This reduction in volume will increase interactions between fibers. From the sequence it is noticed that fibers start to change shape as they contact each other. This effect is due to friction and lubrication forces. As fibers become entangled there is increased contact between them and they eventually start to deform. It is also observed that even for such a simple geometry, fibers are not evenly distributed through the plate as the flow comes to rest.

These specific simulations are currently being used to study the influence of parameters such as fiber length, mold closing velocity and initial mold coverage in weldline development. A second subject of ongoing work is the study of the influence of molding parameters in fiber density distribution. These results will be presented in a future publication.

## Summary and Next Steps

An algorithm that models fiber flow in the molding of polymer composites has been developed. In order to be able to accurately calculate the mechanical properties and possible defects in a finished part it is necessary to account for fiber deformation as fiber flow is influenced by fiber flexibility.

For the case of rigid fibers, the simulation results in general match predictions made with the Folgar-Tucker model for fiber orientation. When modeling the compression molding of thin parts the Folgar-Tucker offers an accurate prediction of fiber orientation within a part. As part thickness increases this prediction starts to be less accurate as the flow becomes three dimensional. It is envisioned that the algorithm developed here can be coupled with existing commercial software for thin compression moldings.

Simulations of the compression molding of SMC have been developed. These simulations provide a better representation of the actual molding process and are able to handle higher fiber volumetric contents. Current work is focused on studying the influence of molding parameters in the development of weldlines and fiber distribution in a molded part.

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