Direct Simulation of Discrete Fiber Suspensions in Polymer Melt Flows

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Discrete fiber polymer matrix composites exhibit significant improvements in thermo-mechanical properties over neat polymers which depend on fiber dispersion and orientation in the final microstructure. Therefore, understanding how these factors evolve during manufacturing and processing is crucial to accurately predict the mechanical response of products made with these materials. For over four decades, orientation tensor-based models have been used to predict fiber orientation of groups of fibers, but underlying assumptions limit the applicability of tensor-based models since they ignore important phenomena such as fiber length distribution, fiber migration, and the effect of spatially varying shear rate on individual fibers. Recently, direct simulation of fibers and fiber suspensions has emerged which are not limited by previous modeling assumptions, but requires careful calibration to accurately represent fiber systems [1]. This study aims to advance the current state of the art for the direct simulation of fibers in polymer melt flows with a goal to improve the accessibility and accuracy of direct fiber simulation while providing enhanced insight into the micromechanics of fiber interactions.

Studies have shown that the behavior of fibers in polymer melt flows is determined by a variety of factors including the physical properties of the fibers, the flow conditions, and the local volume fraction of fibers [2]. The periodic motion of individual isolated fibers in simple shear flow is often described by Jeffery's Orbit and defined through the aspect ratio of the fiber and shear rate of the flow [3]. The change in average orientation of a collection of fibers is typically simulated with tensor-base models initially presented by Advani and Tucker [4] and further expanded to account for more realistic anisotropic rotary diffusion and slowed initial kinematics [5]. The results of these models are determined by fiber aspect ratio, flow shear rates, and choice of closure approximation and diffusion and kinematic parameters. Experiments in fiber composite processing have demonstrated that current fiber orientation models do not accurately represent real systems which are often non-homogenous [2]. Volume fraction and fiber length varies within a given system, which can influence the fiber behavior. Our current focus here is to study the effect of the non-homogeneity of fiber suspensions through direct fiber simulations that may be used to simulate conditions inaccessible to current tensor-based models.

A direct fiber simulation computational approach is developed here that couples Computational Fluid Dynamics (CFD) and Discrete Element Method (DEM) to study the evolution of fiber orientation and volume fraction migration in polymer melt flows. Simulations of a single isolated fiber is considered first where DEM fiber orientation is determined solely by the interaction of fibers with the flow through drag calculations on regularly spaced Flow Sampling Points (FSPs) shown in Figure 1a. The placement of these FSPs $\vec{R}_{FSP}$ is adjusted through an automated surrogate model based calibration process to achieve results in agreement with Jeffery's Orbit. The fiber-fiber interaction for groups of fibers is modeled in DEM (see e.g., Figure 1b) with multiple contact models to capture the change in behavior as fibers approach each other at various speeds, angles, and distances. The parameters of these models are similarly calibrated via surrogate models built with machine learning and the application of optimization techniques to achieve results in agreement with either analytical models or published experimental data [6].

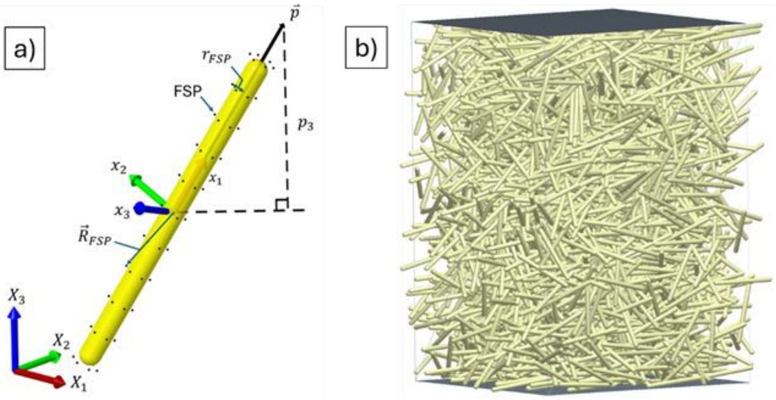

Figure 1: a) A fiber with orientation $\vec{p}$ and Flow Sampling Points used in fiber-flow interaction labeled. b) The simulation domain with a representative collection of individually simulated interacting fibers. [6]

To demonstrate our method, we simulated fibers with an aspect ratio 15.64 and a uniform 8% volume fraction in simple shear with a shear rate of 10 [6]. The analytical model used as the target for calibration was a pARD model with $C_I = 0.0036$ and $\Omega = 0.7$ as the diffusion parameters. The calibration processes produced model parameters that significantly reduced the error in orientation tensor components between our model and the analytical models as shown in Fig. 2 where noteworthy agreement is seen over the entire time history of results. We were able to achieve agreement with Folgar's experimentally obtained steady state orientation distribution for this aspect ratio and volume fraction combination [7] as well. Our model and calibration process perform as well or better than fully custom and proprietary codebases.

Once a calibrated fiber and fiber interaction model are obtained, the direct fiber simulation approach was extended to include bi-directional coupling of the fiber-flow interaction such that the position and orientation of fibers influence the local viscosity and the fluid flow field. Full bi-directional coupling where fibers are individually modeled as geometry in a fine-mesh CFD is computationally expensive, so we periodically utilize spatial averaging of the orientation and volume fraction to enable computationally efficient course mesh CFD that captures the influence of fibers without significantly increasing simulation time. Figure 3 presents preliminary results showing the A_{11} component of the average orientation tensor for two coupled fiber simulations with a Newtonian fluid and a power-law fluid in pressure driven flow between plates for a given flow rate. In these simulations, the pressure gradient is adjusted to maintain a constant average flow rate. As fibers align with the flow and migrate in regions with higher shear rates (i.e. near the walls) the local viscosity decreases and the velocity profile is blunted, resulting in lower shear rates near the center of the flow than would otherwise occur if fibers were not present. This blunting results in slower fiber alignment with the flow in the center of the domain than a uni-directionally coupled simulation under the same conditions. The effect is further exaggerated when a shear thinning fluid power-law fluid model is used as seen in Figure 3b where the central region is less aligned than that in the Newtonian case in Figure 3a.

In other advanced studies, we compute fiber interaction data that cannot be evaluated in current tensor-based models or experimental measurements in order to better understand the underlying physics of fiber behavior. Factors of interest include the strength and frequency of fiber contacts, migration rates of fibers under various flow conditions, and the influence of fiber length distributions. Preliminary results from simulations with length distributions indicate that shorter fibers align less with the flow and have fewer contacts than longer fibers. While direct fiber simulation is computationally more expensive than tensor-based modeling, the method is able to reproduce more realistic conditions and achieve reasonable results while providing enhanced insight that is inaccessible from analytical models or experiments.

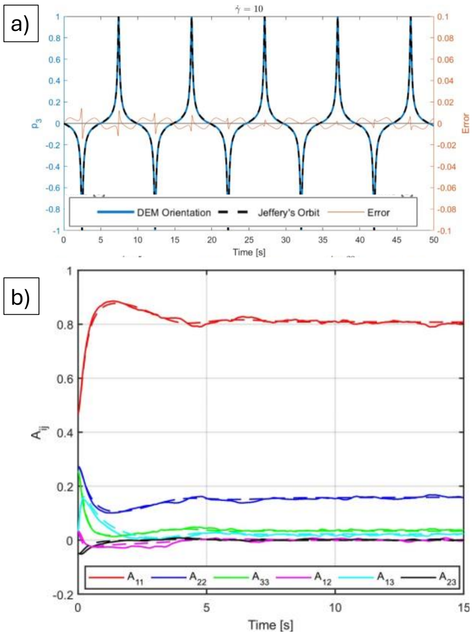

Figure 2: Significant agreement in results from our method (solid lines) and analytical models (dashed lines) for a collection of fibers as compared to (a) a Jeffery's Orbit and (b) a pARD model with $C_I = 0.0036$ *and* $\Omega = 0.7$ [6]

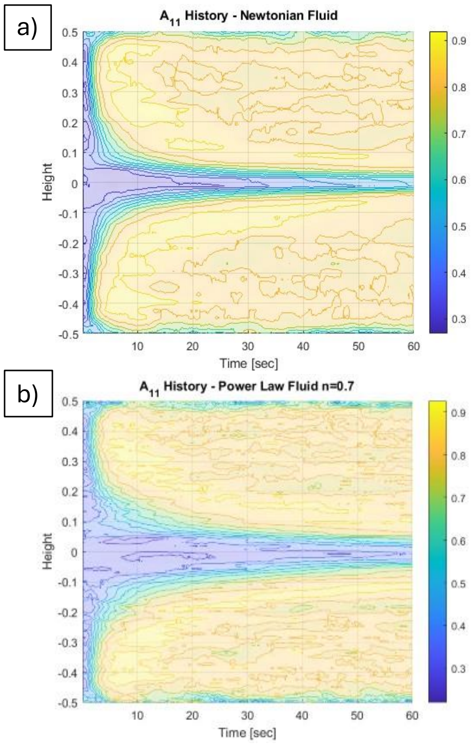

Figure 3: A_{11} orientation component results from viscosity coupled simulation with a (a) Newtonian fluid and a (b) power-law non-Newtonian fluid represented with n = 0.7.

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