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Rheological properties of dilute suspensions of rigid and flexible fibers

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ABSTRACT

Particle-level simulations are used to study the rheology of monodispersed suspensions of rigid and flexible fibers in a creeping, simple shear flow of a Newtonian fluid. We also investigate the influence of different equilibrium shapes (straight and curved) of the fibers on the behavior of the suspension. A parametric study of the impacts of fiber flexural rigidity and morphology on rheology quantifies the effects of these realistic fiber features on the experimentally accessible rheological properties. A fiber is modeled as a chain of rigid cylindrical segments, interacting through a two-way coupling with the fluid described by the incompressible three-dimensional Navier–Stokes equations. The initial fiber configuration is in the flow–gradient plane. We show that, when the shear rate is increased, straight flexible fibers undergo a buckling transition, leading to the development of finite first and second normal stress differences and a reduction of the viscosity. These effects, triggered by shape fluctuations, are dissimilar to the effects induced by the curvature of stiff, curved fibers, for which the viscosity increases with the curvature of the fiber. An analysis of the orbital drift of fibers initially oriented at an angle to the flow–gradient plane provides an estimate for the time-scale within which the prediction of the rheological behavior is valid. The information obtained in this work can be used in the experimental characterization of fiber morphology and mechanics through rheology.

1. Introduction

The dynamics of fiber suspensions is of great interest in many industrial processes, including papermaking [1–3], composites processing [4] and dry-forming of pulp mats. The fiber morphology and flexural rigidity, and the dynamics of the fiber orientation distribution, determine the rheological properties of fiber suspensions [5–11]. The fiber contribution to the stress tensor in dilute and semi-dilute suspension of straight, rigid fibers in a creeping shear flow is relatively well understood [5,12]. Numerous questions, however, arise for systems with any added complexity, including concentrated suspensions, a finite Reynolds number or fiber inertia. Notably, the effects of fiber flexibility and curvature on suspension rheology remain elusive due to the added geometrical complexity of deformable and irregularly shaped fibers. Since the generality of analytical approaches is limited, particle-level simulation techniques represent an attractive alternative for quantifying the relation between the morphological and mechanical properties of the dispersed phase and the stress tensor of the suspension.

The present work is concerned with isolated fibers in a creeping shear flow. A particle-level fiber model is employed to study the rheological properties of the fiber suspension. A novel method is proposed for computing the deviatoric stresses in dilute fiber suspensions from the hydrodynamic forces and torques acting on the fiber segments. This method permits investigation of the effects of the fiber flexibility and fiber shape on suspension rheology. Moreover, this work argues that experimentally accessible rheological properties of the suspension may be used to characterize the morphology and mechanics of the suspended fibers.

Batchelor [5] derived a theoretical expression for the average stress tensor of a suspension from the fiber orientation distribution. The study dealt with elongated rigid particles under the assumption that the particle interactions are only hydrodynamic, i.e. that there are no particle–particle contacts. Jeffery [13] studied the motion of an isolated prolate spheroid in a simple shear flow of a Newtonian fluid. This theoretical study predicts that an ellipsoidal particle rotates in one of a family of repeatable orbits around the vorticity axis, in the absence of particle and fluid inertia. Note that this orbiting behavior yields the fiber orientation distribution of dilute dispersions, which can then be used with Batchelor's

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prediction of the stress tensor contribution of the fibers. Bretherton [14] showed that Jeffery's analysis is valid for any axisymmetric rigid body if an equivalent aspect ratio is used instead of the actual spheroid aspect ratio. The aforementioned theoretical results were derived for straight, rigid fibers.

Particle-level simulations, where fibers are typically treated as chains of rigid bodies, can also be employed to predict the fiber reorientation and the rheological properties of fiber suspension. Matsuoka and Yamamoto [15] developed a particle-level simulation technique to capture the dynamics of rigid and flexible fibers in a prescribed flow field. They represented a fiber by a number of spheres, lined up and connected to each neighboring sphere. Joung et al. [6] proposed a model for flexible fibers where a fiber was modeled as a chain of spherical beads joined by connectors, and the simulations accounted for short and long range hydrodynamic interactions between these beads. Joung et al. [6] investigated the effect of fiber flexibility on the suspension viscosity, and in a later work [7], the influence of curvature of rigid fibers on the suspension viscosity. Ross and Klingenberg [8] modeled a fiber as a chain of rigid, prolate spheroids. They also investigated the transient behavior of the specific viscosity of the suspension in simple shear flow. Schmid et al. [9] developed a particle-level simulation technique to study the flocculation of fibers in sheared suspensions in three dimensions. The fibers were modeled as chains of massless, rigid cylindrical segments interacting with an imposed flow field through viscous drag forces and with other fibers through contact forces. Their study shows that the rheological properties strongly depend on both the fiber flexibility and the equilibrium shape. Switzer et al. [16] employed the particle-level model of Schmid et al. [9] to investigate the impact of the fiber equilibrium shape, the fiber stiffness and the inter-fiber friction on the suspension properties. Lindström and Uesaka [17] further developed the model of Schmid et al. [9], by taking into account the particle inertia, the intermediate to long-range hydrodynamic interactions between the fibers and the two-way coupling between the fibers and the carrying fluid. In a later work, they predicted the rheological properties for fiber suspensions of various volume concentrations, where both hydrodynamic and mechanical fiber interactions were taken into account [10]. They also investigated the effects of the fiber aspect ratio, the fiber concentration, and the inter-particle friction on the stress tensor of a fiber suspension [11]. Wu and Aidun [18] employed a particle-level numerical method to analyze the rheology of flexible fiber suspensions in simple shear flow with a Newtonian medium. They found that the relative suspension viscosity significantly increases when fiber flexibility increases, and that both fiber deformation and fiber–fiber contacts lead to positive first normal stress difference. Salahuddin et al. [19] studied the rheology of semidilute suspensions of rigid fibers in a Newtonian medium. They observed that mechanical fiber–fiber contacts increase both the relative shear viscosity and the first normal stress difference. Recently, Kondora and Asendrych [20] applied a particle-level simulation technique to flexible and rigid fibers in a converging channel of a paper machine headbox, studying the fiber orientation distribution. The fibers were modeled as chains of spheres connected by ball and socket joints.

There are numerous experimental and numerical studies on predicting rheological properties of particle suspensions. However, less attention is paid to determining the properties of the suspended particles from known properties of the suspension. One example is a determination of the size of macromolecules in a dilute solution from the ratio of the viscosity of the solution and the solvent [21]. It is important to realize that a quantitative prediction of the rheological properties of fiber suspensions enables a relatively simple access to mechanical properties of fibers through rheology experiments.

The present work investigates the deviatoric stresses created by the dispersed phase of fiber suspensions, by considering the motion of isolated fibers in a simple creeping shear flow of a Newtonian fluid. Particle-level simulations, based on the model proposed by Lindström and Uesaka [17], are carried out using an open source CFD software [22]. Although both the fiber model and the flow simulations are fully three-dimensional, the initial configuration of the fiber is co-planar with the flow–gradient plane. This choice is made due to extensive previous experimental and theoretical studies in which the fiber motion occurs in the flow–gradient plane [23,24,12]. A parametric study of the orbital drift for the fibers initially oriented at an angle to the flow–gradient plane is performed to identify the time-scale within which the in-plane fiber dynamics is considered stable, and the prediction of the rheological properties is valid. A novel method is proposed for computing the fiber contribution to the deviatoric stresses. The main focus of the work is on the effects of the fiber flexibility and shape on the specific viscosity, and on the first and second normal stress differences.

2. Theory

2.1. Deviatoric stresses of fiber suspensions

A finite volume V of particle suspension that consists of a continuous, Newtonian fluid phase with viscosity η, and a dispersed phase of solid particles, is considered. According to Pal [25], the constitutive equation for a dilute dispersion of solid force-free particles in a Newtonian creeping flow reads

$$\boldsymbol{\sigma} = -p\boldsymbol{\delta} + 2\eta\dot{\boldsymbol{\gamma}} + \frac{1}{V}\sum_{j=1}^{N}\boldsymbol{s}_j. \tag{1}$$

In Eq. (1), $\boldsymbol{\sigma}$ is the volume-averaged stress tensor, $\boldsymbol{\delta}$ is the unit tensor, p is the hydrostatic pressure, $\dot{\boldsymbol{\gamma}}$ is the homogeneous strain rate tensor and N is the number of particles. Furthermore, $\boldsymbol{s}_j$ represents the dipole strength of a single particle, given by

$$\boldsymbol{s}_j = \iint_{S_j}\left[\boldsymbol{\tau}\boldsymbol{r} - \frac{1}{3}(\boldsymbol{r}\cdot\boldsymbol{\tau})\boldsymbol{\delta} - \eta(\hat{\boldsymbol{n}}\boldsymbol{v} + \boldsymbol{v}\hat{\boldsymbol{n}})\right]dA, \tag{2}$$

where S_j is the surface of the jth particle, $\boldsymbol{\tau}$ is the traction vector, $\boldsymbol{r}$ is the position vector of the surface element dA, $\boldsymbol{v}$ is the fluid velocity field, and $\hat{\boldsymbol{n}}$ is the unit outward normal of S_j. For the case of slender particles of circular cross-section, but otherwise arbitrary shape, we have

$$\iint_{S_j}(\hat{\boldsymbol{n}}\boldsymbol{v} + \boldsymbol{v}\hat{\boldsymbol{n}})dA \approx \boldsymbol{0}. \tag{3}$$

This is due to the fact that, when $\boldsymbol{v}$ is essentially constant around the circumference of S_j due to slenderness, the components of the integrated tensor all include a factor $\sin\varphi$ or $\cos\varphi$, with φ being the polar angle of the cross-section. Thus, Eq. (2) reduces to

$$\boldsymbol{s}_j = \iint_{S_j}\left[\boldsymbol{\tau}\boldsymbol{r} - \frac{1}{3}(\boldsymbol{r}\cdot\boldsymbol{\tau})\boldsymbol{\delta}\right]dA. \tag{4}$$

By introducing the number density $n = N/V$, we may write

$$\boldsymbol{\sigma} = -p\boldsymbol{\delta} + 2\eta\dot{\boldsymbol{\gamma}} + n\langle\boldsymbol{s}\rangle, \tag{5}$$

where $\langle\boldsymbol{s}\rangle$ is the ensemble average of the dipole strength.

2.2. Dilute suspensions of straight, rigid fibers

Batchelor considered the deviatoric stresses arising from straight, slender, rigid fibers with length L and aspect ratio r_f. It was found that [5]

$$\boldsymbol{s}_j = \frac{\eta_{fib}}{n}\left(\hat{\boldsymbol{p}}_j\hat{\boldsymbol{p}}_j\hat{\boldsymbol{p}}_j\hat{\boldsymbol{p}}_j - \frac{1}{3}\boldsymbol{\delta}\hat{\boldsymbol{p}}_j\hat{\boldsymbol{p}}_j\right) : \dot{\boldsymbol{\gamma}}, \tag{6}$$