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Effect of fibre curvature on the rheology of particulate suspensions

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This work is dedicated to the memory of Associated Professor Howard See

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ABSTRACT

Rheological properties of non-Brownian straight and curved fibre suspensions in simple shear flow have been investigated by particle-level simulation. An inertialess fibre particle in Newtonian fluid is modelled as a collection of spheres connected with Hookean-type constraint force. The fibre motions are governed by hydrodynamic interaction based on Rotne–Prager correction to velocity disturbance and short-ranged repulsive force. An isolated curved fibre in simple shear flow shows a decrease in the period of rotation with increasing the curvature. Initial stress overshoot is observed as fibres undergo transition from isotropic orientation. Shear viscosity and first normal stress of straight fibre suspensions exhibit scaling with respect to concentration in a manner consistent with comparable literature results. The overall viscosity enhancement with increasing the curvature has been observed over the studied range of aspect ratio and concentration. This is accompanied by the decrease of flow-aligned component of configuration tensor. Straight and curved fibre simulation exhibits an average positive first normal stress difference but the data fluctuation is too large to distinguish curvature effect.

1. Introduction

Fibre suspensions can be found in a wide variety of applications such as pulp and paper production, and composite materials including fibre-reinforced molded plastic and carbon nanotubes composites. Fibre suspensions exhibit complex transient behavior due to flow-induced fibre orientation. The periodic transient behavior can be observed in a simple case of ellipsoid as a representative of fibre-like elongated object. An isolated ellipsoid in a linear flow field undergoes a periodic closed orbit around the vorticity axis while it spends majority of time aligned along the flow direction. This periodic closed orbit is commonly referred as Jeffery's orbit. The periodicity orientation gives rise to oscillating shear viscosity since particle stress is smaller for a spheroid aligned in the flow direction than for a spheroid aligned transverse to the flow. Thus, fibre microstructure has a strong influence on the mechanical properties of suspensions. In some applications such as paper manufacturing, a uniform fibre distribution is preferable for good consistency. On the other hand, the aligned fibre microstructure is a desirable outcome in some fibre-reinforced composite processes. Departure from straight fibre alignment can lead to significant degradation of composite properties [1]. Therefore, it is beneficial for fibre related manufacturing processes to gain insight of the complex interplay between microstructure and the corresponding rheological properties, particularly the impact of particle shape on suspension properties.

Practical fibres are not perfectly straight and tend to deform due to the processing conditions such as exposure to heat source or flow condition. Results of past studies indicate that fibre curvature can significantly affect rheological properties of suspensions. Experimental results of nylon fibre showed that a very slight curvature can produce a large change in viscosity [2]. Switzer and Klingenberg [3] modelled arbitrary-shape fibre as a rigid cylinders with hemisphere end-caps linked by ball and socket joints that allow fibre to bend and twist. Hydrodynamic interactions were treated to be free draining interaction. Short-range repulsive force and mechanical contact force were included in the simulation. Particle-level simulation of U-shaped fibre done by Switzer and Klingenberg [3] demonstrated that a relatively small change from an ideal straight shape results in a large increase of the suspension viscosity. The trend of increasing viscosity for curved fibre is consistent with the finding by Joung et al. [4]. The authors performed a particle-level simulation where fibre was treated as chains of beads linked by connectors. Hydrodynamic interaction was modelled as a superposition of pairwise short-range lubrication and long-range disturbance velocity. Shear viscosity was reported to be larger for curved fibre suspensions than that of straight fibre suspension at the same concentration. Curved fibre with end-to-end curvature between 5° and 10° produced largest shear viscosity. This optimal curvature angle trend was not observed by Switzer and Klingenberg [3].

Fibre hydrodynamics is one the most important modelling feature for non-Browian rigid fibre simulation. A unique hydrodynamics solution is required for each distinct fibre shape. An alternative approach is to construct an arbitary shape fibre from a collection of

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simple shape objects such as sphere whose hydrodynamic solution is commonly known. The idea of fibre model consisting of linked spheres was pioneered by Yamamoto and Matsuoka [5]. The joints between spheres allows for bending, twisting and stretching such that the fibres can assume arbitrary conformation. For rigid fibre, the computed period of rotation and distribution of orientation angle agree with those calculated by Jeffery's equation. Tozzi et al. [6] represented a fibre by a closed-pack shell of spherical bead with the bead center position offsetting below fibre surface. Hydrodynamic interactions between beads were based on Rotne–Prager–Yamakawa approximation. Motion of arbitrary shape fibre could be accurately predicted as demonstrated in the sedimentation case [7]. Larger (intrinsic) viscosity of non-straight fibre suspensions compared to that of straight fibre suspensions is observed in a dilute limit. In this regime, fibre motion is governed entirely by hydrodynamic forces. The intrinsic viscosity is found to be best correlated to an invariant of hydrodynamic derived from a hydrodynamic drag coefficient of fibre. However, bead-shell model can be computationally expensive for a system with large number of fibres in a non-dilute regime. Joung [8] employed a cluster of linked spheres elastically bonded together to form larger rod-like and plate-like particles. Simulation results of isolated particle dynamics in a linear flow field demonstrated Jeffery's orbit periods consistent with theoretical results. The use of linked sphere enables hydrodynamics of non-spherical object to be accounted for in an approximate way using the results for sphere-sphere hydrodynamic force. Kittipoomwong et al. [9] applied the linked sphere concept to model particulate suspensions of various shapes including rod-like and plate-like particle. The inclusion of hydrodynamic interaction led to a shift of orientation distribution toward flow–vorticity plane for rod-like particle similar to experimental observation. The linking of spheres to form a larger structure can be readily extended to model particles of arbitrary shape without incurring a prohibitive computational cost.

In this study, particle-level simulation has been employed to describe relationship between rheological response and fibre shape. We will employ model and simulation method used in Kittipoomwong et al. [9]. Here, particle is modelled as a collection of equal-size neutrally buoyant spheres connected by Hookean-type links. Hydrodynamic interaction is described by pairwise summation of the first reflection of velocity disturbance according to Rotne–Prager tensor. This is followed by discussion of the simulation results. The initial transient response of fibres as they undergo transition from isotropic orientation under shear flow is discussed. The presence of fibre curvature gives rise to several noticeable changes in fibre dynamics properties under shear flow. A single curved rigid fibre in linear flow field exhibits an increasing orbit period with respect to the curvature. Curved fibre is found to spend less time aligning the fibre backbone with the flow. The less likelihood of flow induced alignment also leads to increase in viscosity of curved fibre suspension as compare to straight fibre suspension. First normal stress difference of straight fibre is well characterized by theory proposed by Carter [10]. Finally, main conclusions from this work are summarized.

2. Simulation method

Fig. 1a shows an assembled subunit of eight identical spheres linked together as employed by Joung [8] and Kittipoomwong et al. [9]. Each subunit is linked together in a cubical shape for straight fibre or as a curved segment with the length along fibre backbone (principal direction) varied to form a segment of curved fibre. Then, a curved fibre is constructed by connecting several segments together as illustrated in Fig. 1b. The aspect ratio (a_r) of fibre is defined as the ratio of fibre enveloped length per equivalent diameter. The equivalent diameter is taken to be a diameter of a circle which has the same cross-sectional area to that of fibre cross-sectional area. Here, the fibre volume is approximated by the volume of constituting spheres.

Fibre curvature is characterized by parameter θ denoting the angle of tangent lines between two end segments. The term $180^\circ - \theta$ is zero for straight fibre and increases with fibre curvature. In Fig. 1a, each sphere pair is linked together along the line of centers by Hookean links.

Consider a pair of spheres α and β separated by a distance $r_{\alpha\beta} = \|\boldsymbol{r}_\beta - \boldsymbol{r}_\alpha\|$. The linkage force along the line of centers $\boldsymbol{F}^{\text{link}}_{\alpha\beta}$ on sphere α due to a linkage with sphere β is given by,

$$\boldsymbol{F}^{\text{link}}_{\alpha\beta} = k(r_{\alpha\beta} - r^{\text{eq}}_{\alpha\beta})\boldsymbol{e}_r, \tag{1}$$

where k is the extensional-mode stiffness coefficient, r^{eq} is the equilibrium particle-particle separation distance and $\boldsymbol{e}_r$ is a unit vector along the line from the center of sphere α to the center of sphere β. The bending and twisting motions are ignored. However, the model is capable of reproducing rigid body rotation due to the use of three-dimensional linkage structure.

Suspensions are composed of curved fibre dispersed in a Newtonian suspending fluid of viscosity η_c. Suspensions are exposed to a simple shear flow $\boldsymbol{U}^\infty = (y\dot{\gamma}, 0, 0)$ where $\dot{\gamma}$ denotes shear rate magnitude and y is position along gradient direction. All spheres have radius of a and are considered non-Brownian, neutrally-buoyant and inertialess. In the limit of vanishing particle and fluid inertia, sphere motions are determined by the balance of hydrodynamic force($\boldsymbol{F}^{\text{Hyd}}$) and non-hydrodynamic force ($\boldsymbol{F}^P$) acting on each sphere. The governing equation of sphere α is written as,

$$\boldsymbol{F}^P_\alpha + \boldsymbol{F}^{\text{Hyd}}_\alpha = 0. \tag{2}$$

The non-hydrodynamic force composed of the aforementioned Hookean linkage force in Eq. (1) and short-range repulsive force ($\boldsymbol{F}^{\text{rep}}$). The $\boldsymbol{F}^{\text{rep}}_{\alpha\beta}$ on sphere α due to sphere β is written as,

$$\boldsymbol{F}^{\text{rep}}_{\alpha\beta} = -F^{\text{rep}}_o \frac{\exp(-\kappa(r_{\alpha\beta} - 2a))}{1 - \exp(-\kappa(r_{\alpha\beta} - 2a))}\boldsymbol{e}_r, \tag{3}$$

where κ^{-1} is the decay length, F^{rep}_o is the repulsive force magnitude. The repulsive force calculation is excluded for sphere pairs belonging to the same cluster.

The hydrodynamic force acting on sphere α can be written as [9],

$$\frac{\boldsymbol{F}^{\text{Hyd}}_\alpha}{6\pi\eta_c a} = (\boldsymbol{U}^\infty - \boldsymbol{U}_\alpha) + \sum_{\alpha\neq\beta} \mathbf{M}^{\text{RP}}_{\alpha\beta} \cdot (\boldsymbol{U}^\infty - \boldsymbol{U}_\beta), \tag{4}$$

where $\mathbf{M}^{\text{RP}}$ is the Rotne–Prager tensor and is given by,

$$\mathbf{M}^{\text{RP}}_{\alpha\beta} = \frac{3a}{4r}(\boldsymbol{\delta} + \boldsymbol{e}_r\boldsymbol{e}_r) + \frac{a^3}{2r^3}(\boldsymbol{\delta} - 3\boldsymbol{e}_r\boldsymbol{e}_r). \tag{5}$$

Here, $\boldsymbol{\delta}$ denotes Kronecker delta function, $r = \|\boldsymbol{x}_\beta - \boldsymbol{x}_\alpha\|$, is a separation between sphere α (origin) and sphere β and $\boldsymbol{e}_r = \boldsymbol{r}/r$. To obtain absolute convergent results, the Ewald summed form of $\mathbf{M}^{\text{RP}}$ is used for calculation [11].

Substituting Eq. (4) into Eq. (2) give the governing equation of sphere α motion as:

$$\boldsymbol{U}_\alpha = \boldsymbol{U}^\infty + (6\pi\eta_c a)^{-1}\boldsymbol{F}^P_\alpha + \sum_{\alpha\neq\beta}^{N} \mathbf{M}^{\text{RP}}_{\alpha\beta} \cdot (\boldsymbol{U}^\infty - \boldsymbol{U}_\beta). \tag{6}$$

In principle, an iterative procedure is required to solve for particle velocity $\boldsymbol{U}_\beta$. To improve computational time, the velocity of prior time step is employed as an approximation to the predicted value of $\boldsymbol{U}_\beta$ [12]. The governing equation is non-dimensionalized by the following scale variables: