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Stokesian dynamics simulation of the role of hydrodynamic interactions on the behavior of a single particle suspending in a Newtonian fluid. Part 1. 1D flexible and rigid fibers

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ABSTRACT

As seen in textbooks of polymer physics, a linear polymer chain can be modeled as a filament of connected beads. This concept can also be adapted to fibers and, for example, flexible fibers can be modeled by considering a stretch force, bending and torsion torques with a non-slip condition between adjacent beads, following the particle simulation method. In predicting fiber motions and their relating rheological properties, the importance of hydrodynamic interactions should be analyzed, so in this work we study the effect of hydrodynamic interactions on the behavior of a single flexible fiber under shear using Stokesian dynamics simulation with a $11N \times 11N$ mobility matrix, where N is the aspect ratio of the fiber. Our results indicate that hydrodynamic interaction becomes significant when the fiber is highly flexible.

1. Introduction

Fibrous materials such as rayon, glass, nylon, carbon and so on are commonly used for polymer composites [1]. It is possible to control process ability as well as product quality by controlling the aspect ratio, distribution of aspect ratios, concentration, orientation and states of dispersion and distribution and flocculation and, many researches have focused on structures development under flow both experimentally [2–4] and via simulations.

The most successful model [5,6] for rigid fiber suspensions in a Newtonian fluid was developed based on the Jeffery model [7], considering fiber–fiber interaction and a diffusion term, with which it is possible to predict transient behavior under flow. Combining this with constitutive equations such as those proposed by Dinh and Armstrong [8], Shaqfeh and Fredrickson [9], Hand [10], and by Phan-Thien and Graham [11], it is possible to predict rheological properties. The model has been evaluated by comparing with experimental data, with good results [12].

Most theoretical works on the subject treat rigid fibrous dispersions only, there being quite little theoretical work done on flexible fiber suspensions. An exception is the work by Hinch [13], with which it is possible to predict deformation of a fiber under flow, but not predict fiber tumbling phenomena because of no-thickness of the fiber.

The particle simulation method (PSM) proposed by Yamamoto et al. [14–16], where a fiber is modeled as a connected beads with stretch force, bending and torque torsions and non-slip condition between adjacent beads, was the first research to predict the behavior of flexible fibers under flow. In order to accomplish this, it first applied free-drain approximation [14,15] and then added hydrodynamic interaction [16]. This model has a good potential to explain the relation between structure and rheological properties. For example, fiber deformation induces non-zero first normal stress differences [16].

After PSM higher coarse-grained level models have been proposed to reproduce flexible fiber behavior under flow by Schmid et al. [17,18] and by Switzer et al. [19,20], where a fiber is modeled as a connected rod. In these, each element feels hydrodynamic drag, which is independent from the surrounding elements, that is, a free-draining approximation is applied. By introducing friction in the model, fiber flocculation was predicted.

If a discrete model is applied, hydrodynamic interaction should be considered even for a single fiber because hydrodynamic effects are important in accurately predicting the rheological properties of colloidal suspensions, for instance, shear-thickening [21].

Yamamoto et al. [16] discussed the effect of hydrodynamic interactions under shear for the rigid fiber case by comparing with the predictions of the intrinsic viscosity by the free-drain approximation, and concluded that the hydrodynamic interac-

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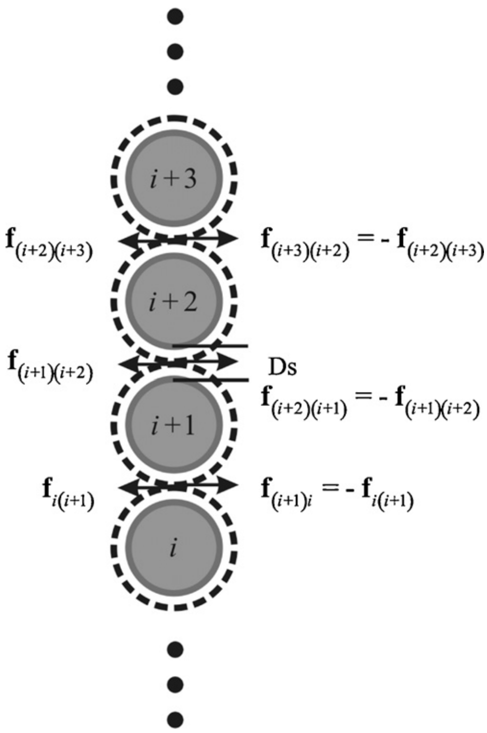

Fig. 1. Fiber model, consisting of a filament of beads with gap.

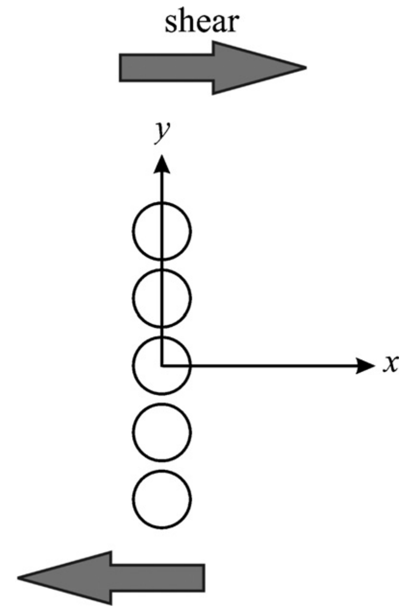

Fig. 2. Initial condition of fiber and shearing direction.

tion becomes important for high aspect ratio fibers. Lindström et al. [22,23] proposed a new model, where an Eulerian formulation, the vorticity-vector potential form of the incompressible Navier–Stokes equations, is used for the fluid, while fibers are modeled as discrete objects interacting with each other through contact forces, and with the fluid through drag forces. The two-way coupling between phases is taken into account by enforcing momentum conservation for fiber–fluid interactions. The authors successfully showed that the first normal stress difference is proportional to the square of the volume concentration of the fibers in the semidilute regime and as concentrations approaches the concentrated regime, it becomes proportional to volume fraction. Joung et al. performed a direct fiber simulation [24], where a fiber is modeled as connected beads considering both lubrication effects and far-field hydrodynamic interactions, and demonstrated that the viscosity of semi-concentrated to concentrated flexible fiber suspensions is higher than that of rigid fiber suspensions.

One of the open questions on flexible fiber suspensions is shear-induced fiber flocculation, for which there are some possible reasons – friction between fibers and hydrodynamic interaction. Schmid et al. [18] reported flocculation resulting from friction only for fibers with a curled equilibrium shape and extremely high friction coefficient. Lindström and Uesaka [23] got shear induced flocculation for straight flexible fiber suspension by considering friction. They suggested that this difference may be from the reduction of penetration of the flow gradient but even now the mechanism is not clear.

PSM considers the hydrodynamic interaction for each fiber and the lubrication approximation between fibers to increase calculating performance. For hydrodynamic interactions, it uses a $6N \times 6N$ mobility matrix, where N is the aspect ratio of the fiber, whereas generally the hydrodynamic interaction considering the disturbance of the deformation rate tensor by surrounding beads [25,26] is described by a $11N \times 11N$ matrix. In order to analyze the importance of hydrodynamic interactions, a PSM-based Stokesian dynamics simulation was performed in this work, but with the full $11N \times 11N$ mobility matrix.

1.1. Fiber and fiber suspension modeling

A PSM-based software was developed by the authors in which a fiber is modeled as a filament of connected beads as shown in Fig. 1. A stretch force $\mathbf{F}^s$, as well as bending $\mathbf{T}^b$, and torsion torques $\mathbf{T}^t$ are considered between adjacent beads. Each of them is described as $\mathbf{F}^s = -k_s(\mathbf{r} - \mathbf{r}_0)$, $\mathbf{T}^b = -k_b(\boldsymbol{\theta}_b - \boldsymbol{\theta}_{b0})$, and $\mathbf{T}^t = -k_t(\boldsymbol{\theta}_t - \boldsymbol{\theta}_{t0})$, respectively, where k_s, k_b and k_t are material constants, $\mathbf{r}$, $\boldsymbol{\theta}_b$, and $\boldsymbol{\theta}_t$ are the position vector, the bending angle, and the torsion angle between adjacent beads, and $\mathbf{r}_0$, $\boldsymbol{\theta}_{b0}$, and $\boldsymbol{\theta}_{t0}$ are the position vector, the bending angle, and the torsion angle at equilibrium state. k_s, k_b and k_t are the spring constants, relating to the Young modulus E and the shear modulus G as $k_s = \pi aE/2$, $k_b = \pi a^3E/8$, and $k_t = \pi a^3G/4$. In this a is the radius of the fiber, i.e., the radius of bead. By varying $\boldsymbol{\theta}_{b0}$ and $\boldsymbol{\theta}_{t0}$, it is possible to treat arbitrary shapes of fiber, such as linear, helical, and so on. In this research, straight flexible fibers are treated, so that both $\boldsymbol{\theta}_{b0}$ and $\boldsymbol{\theta}_{t0}$ are set to 0.

When simulating dynamics of fibers under flow it is important to consider hydrodynamic effects, hydrodynamic force and torque. The simplest method is the free-drain approximation, where each bead experiences a hydrodynamic force $\mathbf{F}^H$ and a hydrodynamic torque $\mathbf{T}^H$, given by Stokes law as

$$\mathbf{F}^H = -6\pi\eta_m a(\mathbf{v} - \mathbf{U}) \tag{1}$$

and

$$\mathbf{T}^H = -8\pi\eta_m a^3(\boldsymbol{\omega} - \boldsymbol{\Omega}), \tag{2}$$

where η_m is the viscosity of matrix, $\mathbf{v}$ and $\boldsymbol{\omega}$ are the velocity and the angular velocity of beads, and $\mathbf{U}$ and $\boldsymbol{\Omega}$ the velocity and the angular velocity of macroscopic fluid flow.

The hydrodynamic effect is affected by the existence of surrounding beads, an effect known as hydrodynamic interaction. The hydrodynamic effect is calculated by [25]:

$$\begin{pmatrix} \mathbf{F}^H \\ \mathbf{T}^H \\ \mathbf{S} \end{pmatrix} = -\mathbf{M}^{-1} \begin{pmatrix} \mathbf{v} - \mathbf{U} \\ \boldsymbol{\omega} - \boldsymbol{\Omega} \\ -\mathbf{E} \end{pmatrix}, \tag{3}$$

where $\mathbf{M}$ is the $11N \times 11N$ mobility matrix, $\mathbf{S}$ is the stresslet and $\mathbf{E}$ is the deformation rate tensor. N is the total number of beads in the systems. If a single fiber is considered, N becomes the aspect ratio