



Dynamics of suspensions of spherical doublets in simple shear and pressure driven flow



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HIGHLIGHTS

- Stokesian Dynamics simulations of bounded flow of concentrated suspension of spherical doublets were performed.
- Rheology and orientation dynamics were studied in shear and pressure driven flows.
- Shear induced migration in pressure driven flow was studied.
- Doublets near the wall were observed to align in the flow direction, whereas in the centre they are randomly oriented.

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ABSTRACT

Suspensions of non-spherical particles are commonly encountered in the flow procedures used in material processing industries and biological applications. The rheological properties of these suspensions are influenced by both the dynamics and the orientation of the suspended particles, which is a characteristic that can be affected by hydrodynamic interactions. The rheology and dynamics of a suspension of spherical doublets in bounded flow between plane parallel walls were examined using the Stokesian Dynamics simulation method. The doublets consisted of two rigid spheres connected by inter-particle forces. These doublets are commonly observed in the agglomeration of particles during the processing of suspensions. The simulations were performed for particles undergoing both simple shear and pressure driven flow between two parallel walls. For all concentrations, the viscosity of the suspension of doublets was observed to be higher than the values determined for spherical particles. The wall normal stresses were similar for both types of suspensions. In addition to the shear and normal stresses, the velocity and concentration profiles in simple shear and pressure driven flow in the channel were also studied. In pressure driven flow, the shear induced migration observed with the doublets was similar to the behaviour observed with the spherical particles. Compared with the suspension of spherical particles in pressure driven flow, the maximum centreline concentration for the doublets always exhibited a lower value. An analysis of the orientation parameter indicated that the doublets near the wall were aligned in the flow direction, with the particles in the centre of the channels exhibiting random orientations.

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1. Introduction

Suspensions of solid rigid particles with various sizes and shapes are encountered in many industrial processes. In many transport processes of practical interest, solid particles can be distinctly non-spherical. In multiple applications, suspended spherical particles can agglomerate, producing doublets and elongated particles that can be distinctly non-spherical. At low Reynolds numbers, a deviation from spherical shapes can often be more important than other particle characteristics. For a suspension of

these particles, the mechanical properties of the final product can depend on the orientation and concentration distribution of the particles. For example, short fibre polymer composites are used in many industrial applications, with the orientation state of the fibres within the polymer matrix determining the material properties of the composite structure. For suspensions of spherical particles, theoretical models exist for predicting multiple physical properties, such as the average sedimentation velocity and the bulk stresses, as discussed in detail in a review article by [Stickel and Powell \(2005\)](#). Determining the dynamics of non-spherical particles can be quite challenging, as theories for the orientation of particles in complex flows have not been well developed. Without a well-developed theoretical model, experiments and computer simulations have been widely used to study the dynamics of the

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suspensions of non-spherical particles. Jeffery (1922) theoretically solved the motion of a single ellipsoidal particle undergoing simple shear flow in a Newtonian fluid. Subsequently, several studies have determined both the rheology and the dynamics of suspensions of elongated particles (Batchelor, 1971; Hinch and Leal, 1976; Lipscomb et al., 1988; Shaqfeh and Fredrickson, 1990). Most of the reports on the suspension of fibres and other shapes of particles have been limited to either infinitely dilute or semi-dilute concentrations that neglect particle–particle hydrodynamic interactions. With increasing particle concentrations, the interactions of a particle with other particles and with the walls of the container can lead to other induced orientations that cannot be explained by Jeffery's results (Moses et al., 2001). Recently, Bertevas et al. (2010) performed simulations of moderately concentrated suspensions of oblate spheroidal particles in a Newtonian fluid, observing that the particles assume preferred orientations that modify both the relative interactions and the stresses in the suspension. Mustafa et al. (2003) experimentally studied the rheological characteristics of non-spherical graphite suspensions, suggesting that both the shape and the processing method can affect the local dispersion conditions.

In addition to the rheology of concentrated suspensions, another phenomenon of considerable interest in the processing of suspensions is shear induced particle migration. The shear induced migration of suspensions with spherical non-Brownian particles has generated considerable interest in the literature (Leighton and Acrivos, 1987; Koh et al., 1994; Phillips et al., 1992; Nott and Brady, 1994; Lyon and Leal, 1998; Morris and Boulay, 1999). These studies have shown that the rate of migration of spherical particles from a high shear rate region to a low shear rate region increases rapidly with increasing particle size. Very few studies on the shear induced migration of suspensions of non-spherical particles have been reported in the literature. Mondy et al. (1994) performed experimental measurements of the concentration profiles generated during shear induced particle migration in suspensions of rods in cylindrical Couette flow and observed a small dependence of the concentration profile on the aspect ratio. Binous and Phillips (1999) studied the effects of sphere-wall interactions on particle motions in both Newtonian and viscoelastic suspensions of dumbbells. The sedimentation of non-spherical particles between two flat plates was also reported in this study, suggesting that a non-spherical particle settling in a channel exhibits an oscillatory motion, but ultimately becomes centred in the channel with the long axis of the particle oriented parallel to gravity. Nitsche and Roy (1996) studied the shear-induced alignment of non-spherical Brownian particles near walls, observing that the steric constraints imposed by the wall can impede the shear-induced alignment near the wall and the particle-wall hydrodynamic interactions act to strengthen the shear-induced alignment near the wall. The hydrodynamic wall effects significantly decreased the rotary diffusivity, with little influence on the angular velocity. Several models for the shear induced particle migration of elongated particles, such as fibres, have been reported. Fan et al. (2000) generalised the diffusive flux model for a suspension of spheres to a fibre suspension and compared the simulation results for circular Couette and plane Poiseuille flow with the experimental results of Mondy et al. (1994). The migration was weak for the fibre suspensions, with a reduced maximum concentration occurring at the centre of the tube for high aspect ratio fibres. Using Stokesian Dynamics simulations, Lopez and Graham (2007) computed the shear induced diffusivities for non-spherical particles with the purpose of evaluating the effects of irreversibility and symmetry breaking. The shear induced diffusivity of rod-like particles was found to decrease with increasing aspect ratios. In contrast with the spherical models, rod-like particles experienced net displacements

from the original streamlines, even in the purely hydrodynamic case. These results suggest a finite value of the diffusivity, even in the absence of repulsive forces between the fibres. Pozrikidis (2005) performed numerical simulations using the boundary element method to study the motion of non-spherical particles suspended in a viscous fluid under conditions of Stokes flow. The simulation results confirmed the occurrence of particle migration due to an effective hydrodynamic diffusivity, illustrating the dependence of the suspension viscosity and the microstructure on the solid-phase areal fraction and the particle aspect ratio. Putz et al. (2010) recently performed simulations of active dumbbell suspensions using the far-field equations of motion valid for dilute suspensions.

The rheology of concentrated suspensions, as characterised by the effective viscosity, concentration dependences and shear induced migration, is of general interest in many industrial applications. In this study, a numerical simulation of a suspension of doublets of spherical particles in wall bounded flows was examined. Considering that the presence of confining walls can significantly affect the suspension rheology and dynamics, most of the numerical simulations on the suspensions of non-spherical particles were conducted with unbounded suspensions. The influence of the walls on these parameters can be less in the interior of the sample, with increasing effects as the confining dimensions become quite small. The doublet particles in our simulations consisted of two spherical beads held together by inter-particle forces. With the simplicity of this formulation, multiple authors have proposed models for elongated particles, such as fibres represented as a chain of spheres. For the most part, these models either considered only far field hydrodynamic interactions that are appropriate for dilute suspensions or included only the lubrication forces present in highly concentrated systems. Stokesian dynamics simulations for concentrated suspensions of doublets in simple shear and pressure driven flow, including both far field and near field hydrodynamic interactions, were performed in this study. In Section 2, the simulation method is described followed by the results in Section 3.

2. Simulation method

The Stokesian Dynamics simulation method (Brady and Bossis 1988) has been used extensively for studying the dynamics of suspensions of rigid spheres in Newtonian fluids in the creeping flow regime. The extension of this method for shear and pressure driven flow of suspensions in a wall bounded system has been provided by Durlafsky and Brady (1989), Nott and Brady (1994) and Singh and Nott (2000). In this work, the approach of Singh and Nott (2000) for the simulation of wall bounded flow was used. This simulation method essentially uses the approach of Nott and Brady (1994) to compute the far-field mobility particle-wall interactions by considering the wall to be comprised of chain of particles. The exact sphere-wall interactions are used for the lubrication interactions between the sphere and the wall in the resistance matrix (Durlafsky and Brady, 1989). The simulation cell used in this present study to perform the dynamic simulations for the bounded flow of suspensions of doublets is shown in Fig. 1. The simulations used two types of particles, wall particles (*W*) and bulk particles (*S*). To simulate simple shear flow, closely packed arrays of wall particles were arranged in top and bottom layers, with the suspended particles positioned between these two layers. The distance between the two layers of the wall particles is termed the Couette gap. To ensure periodic replication in both directions, the simulation cell in the bottom half region contained only pure fluid. The bulk suspension was confined in the gap between the upper wall and the bottom wall in a periodic box. To produce

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