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Migration and chaining of noncolloidal spheres suspended in a sheared viscoelastic medium. Experiments and numerical simulations

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ABSTRACT

Migration and chaining of noncolloidal spheres in a worm-like micellar, viscoelastic solution under shear flow have been studied both experimentally and by numerical simulations. The microstructure dynamics have been experimentally investigated in the flow-gradient and in the flow-vorticity planes. 2D simulations in the flow-gradient plane have been performed for the same geometry, and with a proper selection for the constitutive equation of the suspending liquid. Experimental results show the formation of particle chains in the bulk, along with migration of a considerable fraction of spheres to the walls. At long times, chains in the bulk are stable, and cross-flow migration of individual spheres is suppressed. Numerical simulations with a standard viscoelastic constitutive equation (Giesekus fluid) reproduce the same phenomena observed experimentally, both in terms of fast particle migration to the wall and bulk chain stability. No alignment is, instead, found in simulations with a constant-viscosity, elastic fluid (Oldroyd-B model), in agreement with previous experimental results with Boger fluids.

1. Introduction

1.1. Experimental background

Self-Assembly (SA) of micro- and nano-particles is a relevant and innovative issue in suspension technology [1–9]. Several methods are used for the assembly of spheres in 2D sheets or more complex shapes: specific chemistry with directional colloidal interactions, templating, capillary interactions between particles at interfaces [10], electric and magnetic fields [11,12], to cite a few.

Particles dispersed in complex fluids can be also organized in flow-induced structures, which are determined by the specific viscous and elastic behavior of the suspending medium [7]. In Flow-Induced Self-Assembly (FISA) the resulting microstructures and the self-assembly kinetics depend on the specific rheological response of the fluid and on size, shape and chemical nature of the suspended particles [13,14]. A range of different structures has been observed and studied: strings of spherical particles aligned in the flow direction [13,15–17], 2D sheets of colloidal crystals [18], size-segregated clusters of particles with bimodal size distribution [19]. These structures can form even at very low volume fractions (less than 1%) in non-colloidal, non-Brownian suspensions, where hydrodynamic interactions are the only acting forces.

Earlier experimental studies of FISA in non-colloidal suspensions showed the presence of viscoelasticity-driven sphere alignment in steady shear flow. Whorlow and Highgate proposed that large normal stresses in polymer solutions are responsible for particle chaining [20]. Michele et al. and Lyon et al. both suggested that a critical Weissenberg number (the ratio between the first normal stress difference and the shear stress) of approximately 10 was necessary for chain formation [15,21]. Feng and Joseph investigated particle–particle interaction and microstructure formation in parallel plate flows and suggested that chain formation is due to a dramatic change in the pressure distribution near the particle caused by viscoelastic stresses [22]. Scirocco et al. studied FISA for monodisperse, non-colloidal spheres in different viscoelastic solutions under simple shear flow conditions [13]. They showed that alignment is present in elastic, shear thinning fluids, but not in Boger fluids (elastic, constant viscosity liquids) [13,23], thus proving that large Weissenberg numbers are not a sufficient condition for alignment.

More recently, Pasquino et al. [15–17] studied the shear-induced alignment of non-colloidal spheres in several fluids in the flow-vorticity plane. The kinetics of alignment was quantified by light scattering techniques [15] and by direct optical microscopy. This allowed for the determination of the characteristic time as a function of the flow parameters [17]. The kinetics of string formation in the flow-vorticity plane has also been followed recently by

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Mirsepassi et al. [24] in a custom-made optical shear cell with cone-plate geometry. They studied the cluster size evolution in a slightly shear thinning viscoelastic fluid for a limited set of shear rates.

At the same time scale of alignment, particle–wall hydrodynamic interactions in shear flow have been found to generate migration of isolated particles in a viscoelastic liquid transversally to the main flow direction. In the experiments available in literature, alignment has been always accompanied by migration [13,16]. In a weakly viscoelastic fluid, migration has been proven to appear before alignment occurs on the plates of the flow cell [16].

1.2. Simulation background

Computer simulations are a very useful tool to understand the physical process determining particle migration and assembly in sheared viscoelastic fluids [25–28]. Simulations have typically been restricted to two dimensions. Very few calculations refer to three dimensional flows, because of the heavy computational price.

Recent simulations in confined shear flow [25], supported by experiments [29], showed that the fluid viscoelasticity drives the particle towards the closest wall, regardless of their initial position and of fluid rheology. An imbalance of normal stresses around the particle is suggested to cause cross-flow migration. Since the shear flow is a linear field and, as such, no lateral variation of the shear rate profile is present in the imposed flow field, it is the presence of confining walls to originate the normal stress imbalance.

2D particle structuring in both confined and unconfined viscoelastic shear flow has been recently predicted [26–28,30]. Briels and co-workers have developed and validated the Responsive Particle Dynamics (RaPiD) technique as an efficient method to simulate viscoelastic fluids [28,30], with the capability of handling a relatively large number of colloidal particles in three dimensions when running on a standard desktop computer. As in the 2D case, periodicity was imposed along all directions, thus neglecting wall-induced migration effects. Such 3D coarse grained simulations, however, cannot be easily extended to the case of non-colloidal particles. At present, there is no numerical work including both chaining and migration dynamics.

1.3. Aim of the current work

From the above literature survey, it is clear that several questions about FISA are still open. Among them: are chaining and migration twin phenomena, that is, do they always occur together? Is chaining a wall phenomenon, or chaining is also possible in the bulk? While numerical simulations are able to well describe and predict single particle migration, are they able to mimic the formation of the elongated, chain-like structures observed in experiments? This paper tries to address the above questions by using a combination of FISA experiments and numerical simulations.

Experiments are performed on a very dilute suspension of non-colloidal spheres in a worm-like micellar solution. FISA kinetics is directly obtained from optical microscopy observations in both the flow-vorticity and the flow-gradient planes, under steady and square wave shear flow. In parallel, 2D numerical simulations are carried out by using the Giesekus model as a constitutive equation for the suspending fluid. Simulations are run in such a way as to reproduce the same initial conditions and shear history of the experiments, thus allowing for a direct comparison with the experimental results. To evaluate the effect of the fluid rheology, additional simulations are performed by considering a constant-viscosity, viscoelastic constitutive equation (Oldroyd-B model) as well.

The paper is structured as follows. After this introduction, the material and the experimental techniques, as well as the numerical simulation conditions, are presented. Next, the experimental results are presented and a comparison is made with the results obtained by simulations. Finally, the main results of the work are summarized in the Conclusion section.

2. Materials and methods

2.1. Samples and experimental devices

In the experiments, the suspending medium is a solution of 100 mM cetyl pyridiniumchloride (CPyCl, Merck), 60 mM sodium salicylate (NaSal, Fluka), and 100 mM sodiumchloride (NaCl, Fisher scientific) in demineralized, doubly distilled water. The rheological properties of the suspending fluid at room temperature are shown in Fig. 1. They were measured with a strain controlled rheometer (ARES, TA instruments) by using a cone plate geometry of 50 mm diameter with a cone angle of 0.02 rad. The fluid linear viscoelasticity shows a typical Maxwell behavior, well characterized by a single relaxation time of about 1 s. The flow curve shows a linear behavior for low rates and a stress plateau region when a critical shear rate has been reached. This region is well known to be a fingerprint of a banding instability [31]. The first normal stress difference is non-negligible and its dependence on shear rate tends to be quadratic by decreasing the shear rate.

Monodisperse polystyrene particles (diameter 50 μm, Duke Scientific, cat n°4250A) were first dried out overnight and then dispersed into the fluid by hand-mixing to a volume fraction of 1%. Optical microscopy confirmed that the particles at rest were well dispersed. It was also checked that the sedimentation time-scale was much longer than the experimental time (the density mismatch between particles and fluid is equal to $\Delta\rho = 0.05$ g/cm^3).

The evolution of microstructure was followed in the flow-gradient plane by means of a home-made rheo-optical sliding plates apparatus, described in details elsewhere [32,33]. The samples were sheared in a flow cell consisting of two parallel plates made of optical glass (180 mm × 50 mm × 5 mm). Due to the finiteness of the run of the plate, the flow direction was periodically inverted, i.e., a square wave oscillatory shear flow was imposed. The shear flow in both directions was always applied for 10 s, followed by a 1 s delay necessary for flow inversion.

Observations in the flow-vorticity plane were made by means of a rheo-optical parallel plate transparent flow cell (CSS 450, Linkam) with a transmitted light microscope (Leitz Axioscope 2) coupled to a 12 bit CCD camera (Pantera TF 1M30, Dalsa). The flow-vorticity plane selected for observations was in the middle height of the gap. The microstructure was visualized at a specific radius (7.5 mm from the center of the geometry). The viewing window was 2.5 mm in diameter.

In both geometries the gap was kept at 760 μm, which is more than 15 times the particle diameter. Experiments were conducted at room temperature at the shear rate of 2.5 s^{-1}. In both cases alignment was followed as a function of time. Particles were considered to be aligned in a string when the line that passed through their centers resulted to be parallel to the flow direction, and two consecutive particles are less separated than two particle diameters (see Figs. 2 and 3). A quantitative analysis was performed by a standard image processing and analysis software (ImageJ, freeware, USA). In order to quantify the alignment, we used the following quantity:

$$A_f = \frac{\sum_{L=1}^{L\max} N_L L^2}{\sum_{L=1}^{L\max} N_L L} \tag{1}$$

where N_L is the number of strings that contain L beads. $L = 1$ corresponds to an isolated bead, whereas $L = L_{\max}$ corresponds to the longest string detected in the sample. The alignment factor A_f has