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Numerical simulations of the rheology of suspensions of rigid spheres at low volume fraction in a viscoelastic fluid under shear

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ABSTRACT

We present a 3D numerical investigation of the viscometric functions for suspensions in viscoelastic fluids under steady shear including comparisons with theoretical predictions in the dilute regime and experimental results for non-colloidal suspensions in a Boger fluid. The comparison with dilute suspension theoretical predictions resolves a discrepancy in the literature regarding the second normal stress difference calculated using the Landau–Lifshitz averaging procedure versus using the ensemble averaging procedure. We also determine that the particle contribution to the stress in a dilute suspension in viscoelastic fluids shear-thickens in all viscometric material properties and we present the scaling of the viscometric functions with Weissenberg number (*Wi*). This shear-thickening behavior is fundamentally different from that shown in 2D numerical simulations which are attributed to elongation flow effects between particles. Comparisons with experimental results at volume fraction $\phi = 0.05$, which is the lowest volume fraction available in existing experimental measurements of bulk viscometric functions, highlight the important role of long range hydrodynamic interactions between particles to fully describe the suspension rheology even at low volume fractions. We investigate the effect of hydrodynamic interactions in the flow, vorticity, and gradient directions and show that these interactions can greatly enhance or decrease the viscometric functions as well as change the shear rate dependent behavior of the suspension.

1. Introduction

The dynamics of particle suspensions in viscoelastic fluids is an area of study due to their prevalence in many consumer product industries (filled polymers, paints, foods, coatings, etc.) and other technological applications (drilling muds, fracking fluids, etc.). A deeper understanding of the rheology of such materials would inform better operation conditions, more effective processes, and higher quality products. Because of the industrial relevance of such materials, viscoelastic suspensions have been studied mostly through experiments devoted to concentrated suspensions. However, due to the diverse nature of viscoelastic fluids and the nonlinearity of the stress-strain relationship in such systems, a deeper fundamental understanding of viscoelastic suspensions is challenging and unfortunately lacking. Few theoretical results exist and these predictions are often only valid in a flow regime (i.e. very "weak" flow and infinite dilution) difficult to observe experimentally. Moreover, the theoretical results for dilute suspensions of torque-free, force-free rigid spheres in a weakly non-Newtonian fluid are still a matter of controversy at the time of this writing [1–5]. Numerical tools for computing the rheology of viscoelastic suspensions are few and most have focused on 2D, which do not provide a complete picture and often differ qualitatively and quantitatively from experiments [6,7]. As such there is a need for 3D simulations to probe the theoretical calculations and provide a fundamental understanding of the mechanisms present in rheological experiments.

In this paper, we focus on viscoelastic suspensions in a simple shear flow. Shear flow is widely used to test the mechanical response of a complex material. Several experimental papers have been published in this area, with different suspending fluids and sizes or shapes of the filler particles [8–16]. We limit our interest to viscometric functions for non-colloidal suspensions of spheres in Boger fluids, since our primary goal is to gain insight into the effect of fluid elasticity on the rheological behavior of suspensions. Specifically, we will make numerical simulation comparisons to the data by Dai et al. [16]. There are several interesting observations

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from the experimental data. First, though the suspending Boger fluid is of constant shear viscosity, suspensions exhibit mild shear-thickening (e.g. in the shear viscosity) at higher shear rates even at the lowest particle volume fraction tested, $\phi = 0.05$. Similarly, shear-thickening behavior was observed by Scirocco et al. in Boger suspensions with a particle volume fraction as low as $\phi = 0.07$ [13]. This is actually the opposite of what is observed in Newtonian fluids, where the viscosity of suspensions tend to shear-thin for larger volume fractions ($\phi > 0.3$) due to particle surface interactions [17]. 2D simulations of viscoelastic suspensions report conflicting results for the bulk viscosity depending on the relative solvent and polymer contributions [6,7]. Second, the viscometric functions measured for $\phi = 0.05 - 0.4$ show increases with ϕ that are larger in magnitude than the theoretical predictions from dilute theory [16]. Thus, one can anticipate that even at $\phi = 0.05$ it is crucial for the role of multibody interactions to be resolved in order for theoretical or numerical work to be experimentally relevant. Another concern lies in existing measurements of the second normal stress difference. Experiments with Boger fluids show that the bulk second normal stress difference is always negative for the suspensions [16]. However, the published particle correction to the second normal stress is negative using the Landau–Lifshitz averaging method [3,4] but positive using the ensemble averaging method [1,2,5]. The theoretical calculations have not been verified numerically and, given that long range hydrodynamic interactions play a role in these suspensions, it is unclear whether the predictive failure lies in the type of averaging procedure or in the neglected particle-particle interactions. Currently, few numerical tools are available to tackle this problem. D'Avino et al. performed 3D simulations of viscoelastic suspensions of spheres under small and large amplitude oscillatory shear but they were limited in the number of cycles that they could handle and could not determine the effect of structure formation at longer time scales [21]. No other 3D simulations of the rheology of viscoelastic suspensions exist to our knowledge.

We present a numerical study of viscoelastic suspension rheology using a 3D parallel code based on an unstructured finite volume formulation for incompressible flow. The viscoelastic suspending fluid is described using the Giesekus constitutive model, which is fit to a number of existing Boger fluid rheologies. We show that the discrepancy in the dilute theory predictions is not a result of differences in averaging procedure but instead inaccurate calculations of the change in the polymer fluid stress due to local disturbances induced by the particles. We also studied dilute suspensions as a function of *Wi* and found that the particle contribution to all viscometric functions exhibit shear-thickening. Using these results we have determined the leading order *Wi* corrections (for $Wi << 1$) to the viscosity, first normal stress difference coefficient, and second normal stress difference coefficient for dilute suspensions in an Oldroyd-B fluid. Comparison between dilute suspension simulations and experimental measurements at low volume fractions was unsatisfactory so we also studied hydrodynamic interactions in the flow, vorticity, and gradient directions to gain insight into the effect of such interactions on the rheology of non-dilute suspensions. We hope that the studies presented will direct further fundamental investigations of suspensions in viscoelastic fluids and inform models to describe higher suspension concentrations.

2. Numerical methods and validation

2.1. Problem definition and governing equations

We consider a neutrally buoyant torque-free and force-free sphere in a shear flow applied across the x-y plane of the computational domain, which has periodicity in the x and z directions

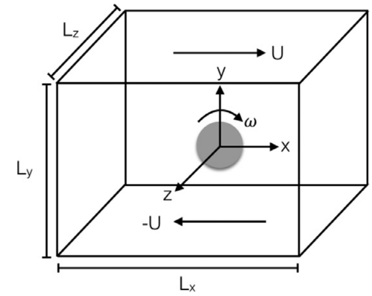

Fig. 1. Schematic of the computation domain.

(cf. Fig. 1) to study dilute suspensions and hydrodynamic interactions.

The sphere is located at the center of the domain and shear flow is applied by moving the walls (located at $y = \pm L_y/2$) at equal and opposite velocities $\pm U$ in the x direction. The simulations are completed by solving the continuity and momentum equations for the flow of an incompressible fluid containing polymer additives around the sphere:

$$\nabla \cdot \mathbf{u} = 0 \tag{1}$$

$$Re \frac{D\mathbf{u}}{Dt} = -\nabla p + \beta \Delta \mathbf{u} + \nabla \cdot \mathbf{\Pi}, \tag{2}$$

where $\frac{D}{Dt} = \frac{\partial}{\partial t} + u \cdot \nabla$. Here the velocity scale is taken as $\dot{\gamma} a$ where a is the particle radius and $\dot{\gamma} = 2U/L_y$ is the imposed shear rate. Stresses are nondimensionalized by $\eta_0 \dot{\gamma}$ where η_0 is the zero-shear viscosity of the fluid. The Reynolds number *Re* is defined as $\rho \dot{\gamma} a^2/\eta_0$ and describes the relative importance of inertial forces to viscous forces. In the zero shear limit the fluid is Newtonian (see Eqs. 3 and 5), with the polymer contribution to the viscosity defined as η_p and the solvent contribution as η_s. Thus $\eta_0 = \eta_s + \eta_p$ and $\beta = \eta_s/\eta_0$.

To describe the polymer stress, $\mathbf{\Pi}$, we implement the Giesekus constitutive equation, which can be written as:

$$\mathbf{\Pi} = \frac{1-\beta}{Wi}(\mathbf{c} - \mathbf{I}) \tag{3}$$

$$\frac{D\mathbf{c}}{Dt} - \{(\nabla \mathbf{v})^T \cdot \mathbf{c} + \mathbf{c} \cdot \nabla \mathbf{v}\} = -\frac{1}{Wi}(\mathbf{c} - \mathbf{I}) - \frac{\alpha}{Wi}(\mathbf{c} - \mathbf{I})^2, \tag{4}$$

where $\mathbf{c}$ is the conformation tensor, α is the anisotropy or mobility parameter, and $Wi = \lambda \dot{\gamma}$ is the Weissenberg number (λ is the polymer relaxation time). When $\alpha = 0$, we recover the Oldroyd-B constitutive equation. It is also well known that in the limit of small *Wi*, we recover the behavior of a second-order fluid (SOF) [22]

$$\boldsymbol{\sigma} = \boldsymbol{\gamma}_{(1)} - Wi\{(1-\beta)\boldsymbol{\gamma}_{(2)} + \alpha(1-\beta)\boldsymbol{\gamma}_{(1)} \cdot \boldsymbol{\gamma}_{(1)}\} \tag{5}$$

$$\boldsymbol{\gamma}_{(1)} = \nabla \mathbf{v} + (\nabla \mathbf{v})^T \tag{6}$$

$$\boldsymbol{\gamma}_{(2)} = \frac{D\boldsymbol{\gamma}_{(1)}}{Dt} - \{(\nabla \mathbf{v})^T \cdot \boldsymbol{\gamma}_{(1)} + \boldsymbol{\gamma}_{(1)} \cdot \nabla \mathbf{v}\} \tag{7}$$

2.2. Bulk stress

We are interested in determining the particle contribution to the bulk stress in a suspension. Since the stress varies with time and position in a suspension, the bulk stress only makes sense as an averaged quantity [32], i.e. averaging the stress at a point in the domain over many different realizations of the suspension or "ensemble averaging". If the statistical properties of the suspension do