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Small- and large-amplitude oscillatory rheometry with bead–spring dumbbells in Stokesian Dynamics to mimic viscoelasticity

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ABSTRACT

In many areas of suspension mechanics, such as filled polymer fluids or household products such as toothpaste, the suspending fluid itself is inherently non-Newtonian and may exhibit viscoelastic properties. In this paper, we extend the Stokesian Dynamics formalism to incorporate a simple model of viscoelasticity by using small spheres as 'beads' in a bead–spring dumbbell (such as is found in the derivation of Oldroyd and FENE constitutive models for dilute polymer solutions). Various different spring laws are then tested in both small-amplitude and large-amplitude oscillatory shear, and their rheological behaviour is compared to continuum constitutive models.

1. Introduction

Suspensions of particles in fluids can be found both in nature and as the basis of many products in industry. Blood, ceramics, paper pulp, paint and adhesives, to name just a few, can all be characterised as a background fluid in which small particles are distributed. A popular simulation technique for these suspensions is Stokesian Dynamics [1]: a microhydrodynamic, low Reynolds number approach to modelling suspensions which considers the interaction of particles with each other against a Newtonian background solvent. Typically it is chosen for its suitability for three-dimensional simulation with low calculation and time penalty.

However, in many areas of suspension mechanics, the suspending background fluid itself is inherently non-Newtonian and may exhibit viscoelastic properties. A sensible step, then, is to extend the Stokesian Dynamics formalism to incorporate a simple model of viscoelasticity. As first seen in Binous and Phillips [2], we do this by using small spheres as 'beads' in bead–spring dumbbells.

Having done this, we observe the performance of these dumbbell suspensions in simulation by submitting them to oscillatory shear. Oscillatory rheometry, both with small-amplitude shear and large-amplitude shear, has become a standard tool in the classification of viscoelastic fluids [3]. We can compare the measurements from the simulations under oscillatory shear with established constitutive models and experimental results from the literature to establish the validity of this extension of the Stokesian Dynamics method.

Alternative simulation techniques for viscoelastic suspensions have been developed, using finite element [4], finite volume [5], and fictitious domain methods [6], as well as methods which treat all suspended particles as passive, allowing the fluid flow to be computed separately [7]. These methods require meshing a (normally periodic) domain, which can place computational limits on the size of the domain and the smallest particle size. Stokesian Dynamics does not require meshing, and so can offer larger domains, a wider choice of particle sizes, flexibility with geometry—walls can be created from fixed particles—and different imposed flows.

In Section 2 of this paper, we summarise the theory of oscillatory rheometry and describe how we extend the Stokesian Dynamics formalism to incorporate the bead–spring dumbbell model of viscoelasticity. We then describe how we extract the rheological measurements from our simulations. In Section 3, we compare the behaviour of different spring laws under small-amplitude oscillatory shear, while in Section 4, we compare different models under large-amplitude oscillatory shear. In both of these sections, we investigate the effect of altering the parameters in the model, and compare their rheological behaviour to continuum constitutive models.

2. Linear rheological measurements

2.1. Theory

Ideal rheometrical measurements are taken in simple shear, or viscometric, flow,

$$\boldsymbol{u} = (\dot{\gamma} y, 0, 0), \qquad \dot{\gamma} = \frac{\mathrm{d}u}{\mathrm{d}y}. \tag{1}$$

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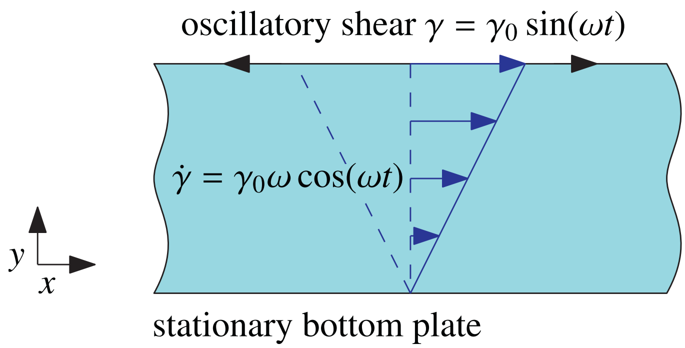

Fig. 1. Oscillatory shear flow.

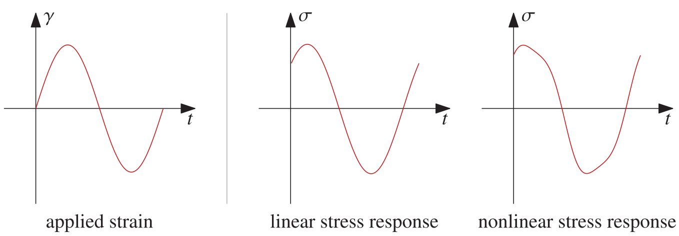

Fig. 2. A linear and nonlinear stress response to an oscillatory shear over time. For SAOS, we expect the former, but for LAOS, we expect the latter.

In a linear viscoelastic fluid, the stress response to this applied shear is dictated not just by the current rate of strain, but also by historical rate of strain,

$$\sigma(t) = \int_{-\infty}^{t} G(t-t')\dot{\gamma}(t')\,\mathrm{d}t'. \tag{2}$$

The function $G(t)$ is the relaxation modulus of the fluid, and represents the importance of the rate of strain from a time t ago on the current stress in the system. Determining the form of the relaxation modulus is the goal of linear rheology, as it allows for the classification of viscoelastic fluids. For example, a purely viscous fluid of viscosity η has a relaxation modulus of $G(t) = \eta\delta(t)$, where $\delta(t)$ is the Dirac delta function, and a linearly elastic solid has a constant relaxation modulus: $G(t) = G_0$.

The relaxation modulus of a fluid can be determined by applying oscillatory shear, where the shear, γ, and shear rate, $\dot{\gamma}$, are given by

$$\gamma(t) = \gamma_0\sin(\omega t), \qquad \dot{\gamma}(t) = \gamma_0\omega\cos(\omega t), \tag{3}$$

for an amplitude γ_0 and frequency ω.

This can be realised in experiments by placing the fluid in a Couette cell and rotating the inner cylinder so as to impose a shear on the fluid. So long as the gap is narrow compared to the cylinder radii, and there are no instabilities or shear inhomogeneities, this is equivalent to simple shear flow (Fig. 1). In practice the amplitude of the oscillation must be small enough so that the stress response of the fluid is also sinusoidal, i.e. the fluid must remain in its linear regime. At these amplitudes the stress is linear in the amplitude [3]. These tests are called small-amplitude oscillatory shear (SAOS).

If the amplitude is increased, the stress response of a fluid may no longer be sinusoidal. For these large-amplitude oscillatory shear (LAOS) tests, a typical nonlinear response is demonstrated in Fig. 2. Although the following definitions are only defined for small-amplitude oscillatory shear, their large-amplitude analogues provide useful rheological data [3], as discussed in Section 4.

Imposing an oscillatory shear, Eq. (3), if we stay in the linear regime the stress can be written as [8]

$$\sigma(t) = G'\gamma(t) + \frac{G''}{\omega}\dot{\gamma}(t), \tag{4}$$

where G' is the storage modulus and G'' the loss modulus. This form is powerful because it splits the viscous and elastic contributions: the storage modulus G' is associated with the total shear γ, and thus represents elasticity. The loss modulus G'' is associated with the instantaneous shear rate $\dot{\gamma}$, and thus represents viscosity.

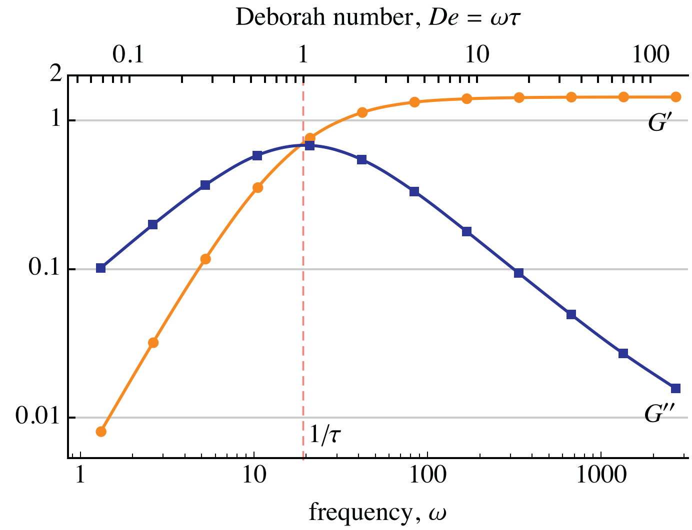

Fig. 3. A typical plot of G' and G'' for a viscoelastic fluid—here, the Oldroyd-B fluid we investigate in Section 3.2—at different frequencies. The inverse of the frequency where the curves intersect, τ, is described as the typical relaxation time of the fluid, and defines where the Deborah number, $De = \omega\tau$, is 1.

The two moduli G' and G'' are measured by rheologists as a function of frequency, ω, for a wide range of viscoelastic fluids. A typical example is shown in Fig. 3. The inverse of the frequency where the two curves intersect, $\tau = 1/\omega_{\text{intersect}}$, is described as the typical relaxation time of the fluid. This parameter allows us to nondimensionalise Eq. (3) [9], writing the imposed shear as

$$\gamma(t) = \frac{Wi}{De}\sin\left(De\,\frac{t}{\tau}\right), \tag{5}$$

where the Deborah number, $De = \tau\omega$, is the ratio of the relaxation time to the oscillation period, and the Weissenberg number, $Wi = \tau\gamma_0\omega$, is the ratio of viscous forces to elastic forces. However, since determining τ requires us to have already determined G' and G'', we choose not to nondimensionalise the equations in this way.

2.2. System details for simulations

In this paper we perform oscillatory simulations on a sample of Newtonian fluid with dumbbells suspended in it. We implement the dumbbells in Stokesian Dynamics as pairs of small spheres (with radius $a = 1$ in our choice of units), a variable distance apart, with a force between the two. We place our dumbbells in a periodic box of side length 150 units. The dumbbells are constrained to lie in a plane, 2 units deep, so that our simulations are carried out on a monolayer of particles. The method remains three-dimensional.

To stop the dumbbells contracting to zero length in an otherwise quiescent flow, the dumbbells are given a natural length of $L = 20$, with which they are initialised. We later vary the number of dumbbells in the sample, but unless otherwise stated, we use an area concentration of 10%. The suspension undergoes eight shear periods, with the number of timesteps per period ranging from 80 to 1200, depending on the frequency and amplitude of shear; see discussion in Section 3.2. The final shear period is used for our analysis; and we use the ensemble average of three independent solutions.

The use of dumbbells in Stokesian Dynamics was first seen in Binous and Phillips [2], where a relationship was formulated between the dumbbells' velocities and the forces exerted on them. In our implementation for small-amplitude oscillatory shear, we go further by letting beads interact with each other through lubrication, allowing us to examine concentrated suspensions. No non-hydrodynamic forces on the beads