

Irreversibility and chaos: Role of lubrication interactions in sheared suspensions

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We investigate non-Brownian particles suspended in a periodic shear-flow using simulations. Following Metzger and Butler [*Phys. Rev. E* **82**, 051406 (2010)], we show that the chaotic dynamics arising from lubrication interactions are too weak to generate an observable particle dispersion. The irreversibility observed in periodic flow is dominated by contact interactions. Nonetheless, we show that lubrication interactions must be included in the calculation to obtain results that agree with experiments.

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I. INTRODUCTION

Viscous suspensions of non-Brownian and neutrally buoyant spheres in a periodic shear flow exhibit a remarkable transition. At a given volume fraction, if the strain amplitude surpasses a critical value, the suspension transitions to a fluctuating state: the particles do not return to their original positions and when tracked stroboscopically at the end of each cycle of shear, the particles exhibit large fluctuations analogous to a random walk [1–4].

This dispersion of particles has attracted a large interest since sheared suspensions often are assumed to be governed by reversible equations (Stokes equations). Within this “pure-hydrodynamic limit” (i.e., only hydrodynamic forces are present and the Reynolds number is zero), the irreversible motion of the particles was attributed to the chaoticity of the hydrodynamic interactions [2,5,6]. Chaos, when coupled to any source of noise, ensures that reversing the direction of flow does not in practice lead to a time-reversed motion for all of the particles; any small perturbation in the state of the system grows exponentially in time. Thus, according to this explanation, small perturbations (weak Brownian motion, particle roughness, or any finite-ranged force), which are inevitably present in real suspensions, are amplified and give rise to the observed particle dispersion.

However, other studies have shown that the extent of irreversibility in concentrated suspensions strongly correlates with the particles’ roughness [7–9]. Similar observations were reported for very dilute suspensions [10] and for the interaction between two particles [7,11], where chaos cannot explain the lack of reversibility.

Thus, fundamental questions persist regarding the role of the hydrodynamic interactions and whether contacts should be considered just a source of noise or as a primary source of irreversible displacements. The suspension dynamics arise from three different contributions: (i) the long-range hydrodynamic interactions, (ii) lubrication, which results from the thin layer of viscous fluid that separates nearly touching particles, and (iii) contacts, which prevent particles from overlapping. It is difficult from experimental results or from existing numerical simulations (Stokesian dynamics) to discern which mechanism causes the irreversibility, as all three contributions are present at the same time.

Resolving the questions requires separating the different contributions to the particle dynamics and estimating

their relative importance. This systematic approach already demonstrated that the long-range hydrodynamic interactions are not a source of chaos and are not responsible for the observed irreversibility [1]. The present work continues this investigation by probing the role of hydrodynamic interactions between particles at short range: the lubrication interaction.

II. MODEL

A minimal model was developed to inquire specifically about the role of lubrication in generating chaotic and irreversible behavior in sheared suspensions. A total of N particles is initially distributed in a square box with nonoverlapping positions to give an areal-fraction ϕ ; simulating a monolayer of particles provides substantial savings in computational time while maintaining an accurate description of the relevant physics. The particle positions are periodic in the flow, or x , direction and are constrained in the gradient, or y , direction by solid walls. In the absence of inertia, the sum of the hydrodynamic forces, \mathbf{F}_i^h , and the contact forces, \mathbf{F}_i^c , on each particle i balance,

$$\mathbf{F}_i^h + \sum_{j \neq i}^N \mathbf{F}_{ij}^c = 0. \quad (1)$$

The hydrodynamic forces are given by

$$\mathbf{F}_i^h = 3\pi\mu d(\mathbf{u}_i - \mathbf{u}_{i\infty}) + \sum_{j(i)} \frac{3\pi\mu d^2}{8h_{ij}} \mathbf{n}_{ij}(\mathbf{u}_i - \mathbf{u}_j) \cdot \mathbf{n}_{ij}, \quad (2)$$

where μ denotes the fluid viscosity, d the particle diameter, and \mathbf{u}_i the velocity of particle i . The fluid velocity at $\mathbf{x}_i = (x_i, y_i)$, the position of particle i , is $\mathbf{u}_{i\infty} = \dot{\gamma} y_i$ and $\dot{\gamma}$ is the shear rate. Lubrication forces between particle i and the particles $j(i)$ located within the lubrication range of particle i depend upon the relative velocities and separation distance $h_{ij} = |\mathbf{x}_{ij}| - d$, where $|\mathbf{x}_{ij}| = |\mathbf{x}_i - \mathbf{x}_j|$, of each pair. The particles $j(i)$ located within the lubrication range of particle i satisfy $2\epsilon_r \leq h_{ij} \leq d/2$, where ϵ_r is the particle roughness. The algorithm only accounts for the normal component of lubrication [12], which acts along the particles’ common normal, $\mathbf{n}_{ij} = \mathbf{x}_{ij}/|\mathbf{x}_{ij}|$. The contact forces are given by

$$\mathbf{F}_{ij}^c = \begin{cases} F_0 \mathbf{n}_{ij} & \text{if } |\mathbf{h}_{ij}| \leq 2\epsilon_r \\ 0 & \text{if } |\mathbf{h}_{ij}| > 2\epsilon_r, \end{cases} \quad (3)$$

where F_0 denotes the amplitude of the repulsive force. We set $F_0 = 3\pi\mu\dot{\gamma}dH$, where H is the separation distance between the shearing walls, and ϵ_r was varied between 0 and $10^{-2}d$.

The equations presented above are solved for the velocities of the particles given their spatial positions. The positions are updated in time using a fourth-order Runge-Kutta method with a time step that ensures a displacement of less than $d/200$ for every particle. Simulations were performed with up to $N = 50$ particles that were tracked over a strain $\gamma = 10$ for continuous shear simulations. One strain unit corresponds to a relative displacement of the cell walls equal to their separation distance. We also performed simulations applying a periodic shear with strain amplitudes γ_0 between 0.5 and 6 and a total accumulated strain of 400. The total accumulated strain after n cycles is $\gamma = 4n\gamma_0$, as γ_0 is the strain for a quarter-cycle.

Equations (1)–(3) describe a sheared suspension of particles interacting through lubrication and contact forces. The model does not include long-range hydrodynamic interactions purposely, as we aim to investigate whether lubrication forces engender chaotic and irreversible behavior. The investigation is facilitated by simulating three different conditions: (i) the “pure lubrication limit,” in which case the contact force and roughness are set to zero, $F_0 = 0$ and $\epsilon_r = 0$; (ii) the “pure contact limit,” where the lubrication forces are not included; and (iii) simulations containing both lubrication and contact forces.

III. RESULTS

We first investigate the relative trajectory between two particles as calculated for the three different cases. The results, shown in Fig. 1, are compared to the full-solution obtained by integrating the equation of da Cunha and Hinch [13], which includes the long-range hydrodynamic interaction. The trajectory obtained with lubrication differs from the full-solution: deviation of the trajectory occurs only when the particles are very close (within the lubrication range). However the symmetry, and thus reversibility, of the trajectory is preserved. The minimum separation distance between the two particles is $h_{12} = 3 \times 10^{-6}d$. Similar to the observation of da Cunha and Hinch [13], the trajectory becomes asymmetric when the contact force is included and the minimum separation distance falls below $2\epsilon_r$. Including the contact force and ignoring lubrication results in an even larger asymmetry of the trajectory, as the motion of the particles follows the streamlines of the background shear flow after contacting.

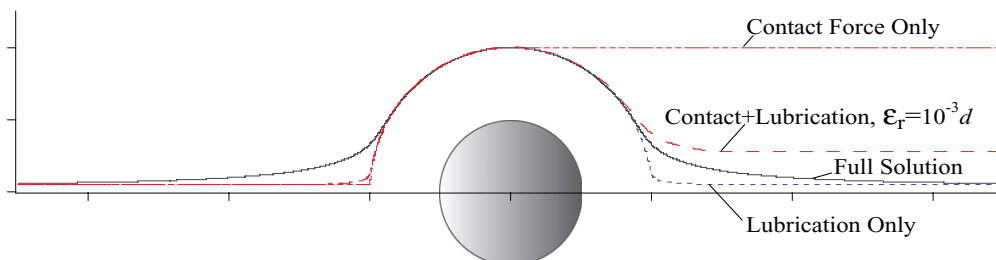


FIG. 1. (Color online) Relative trajectory between two particles initially located at $(x_1, y_1) = (0, 0)$ and $(x_2, y_2) = (-10, 0.1)$.

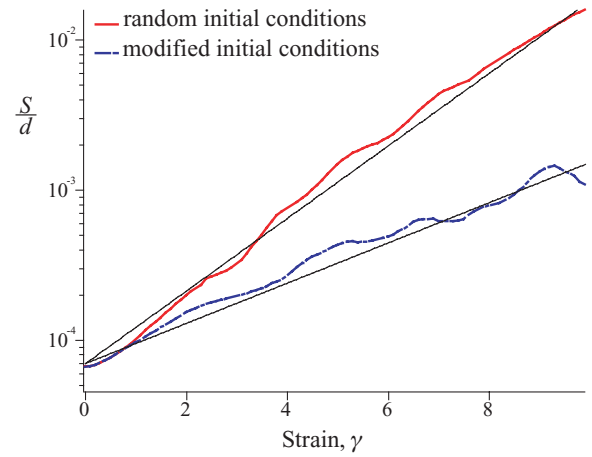


FIG. 2. (Color online) Separation distance, S , versus strain obtained in the “pure lubrication limit” ($F_0 = 0$) for $N = 50$, $\phi = 0.25$, and a steady shear flow.

Note that the equations can also be integrated for small total strains for multiple particles in the “pure lubrication limit” without violating the excluded volume restrictions. This allows us to investigate whether lubrication interactions alone lead to chaotic dynamics. Following Refs. [1,14–16], two random distributions of 50 particles each are simulated. The second distribution, labeled B, is prepared from the original configuration, labeled A, by displacing each particle in a random direction by a small distance $\epsilon = 10^{-4}d$. The Euclidian distance between these two simulations is computed in phase space as $S = \sqrt{\frac{1}{N} \sum_{i=1}^N (y_i^A - y_i^B)^2}$ [18]. For chaotic systems, S grows exponentially as $\epsilon e^{\lambda\gamma}$, where λ is the Lyapunov exponent. Figure 2 shows the exponential increase of the separation distance, S , with accumulated strain amplitude, γ . The positive value of the Lyapunov exponent, $\lambda = 0.56$, is a clear indicator of chaos. The separation distance was obtained by averaging data from nine sets of simulations.

We can identify two distinct mechanisms that potentially contribute to the amplification, seen in Fig. 2, of the initial perturbation. One contribution is from the N -body dynamics occurring through the lubrication interactions. The second is a two-body mechanism arising from the strong focusing and defocusing of streamlines, which is illustrated in Fig. 3(a). Two particles placed on top of each other separate on very different streamlines if a small perturbation is imposed on their initial position; see Fig. 3(b). We systematically quantify this effect by measuring the amplification factor, α/ϵ , where α and ϵ are the final and initial distance between these two streamlines,

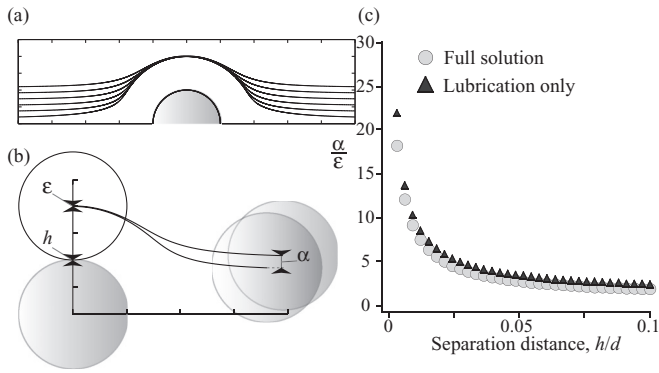


FIG. 3. (a) Illustration of the streamline focusing and defocusing before and after the apex of the interaction. (b) Relative trajectories for two particles initially displaced at $[(x_1, y_1) = (0, 0), (x_2, y_2) = (0, d + h)]$, and at $[(x_1, y_1) = (0, 0), (x_2, y_2) = (0, d + h + \epsilon)]$, with $h = 5 \times 10^{-4}d$ and $\epsilon = 5 \times 10^{-4}d$. The distance in the y direction between these two trajectories after a strain $\gamma = 10$ is α . (c) Amplification caused by the streamline defocusing, α/ϵ , versus initial separation distance, h .

respectively, as the function of the initial particle separation distance h . Figure 3(c) shows that the amplification of an initial perturbation can be $O(20)$ for two particles initially separated by a small distance h . However, this effect decreases when the initial separation distance increases; two particles initially separated by a distance $h > 0.1d$ are weakly sensitive to this mechanism as $\alpha/\epsilon \rightarrow 1$. Note that this amplification is the same using the full solution of da Cunha and Hinch [13] or lubrication only.

To remove this effect in the estimation of the Lyapunov exponent, simulations were performed with altered initial conditions where the minimum separation distance between particles was set at $0.1d$ instead of zero. The results calculated from these initial conditions, labeled as “modified initial conditions” in Fig. 2, show that S still grows exponentially, albeit with a lower rate of $\lambda = 0.31$. The lubrication interactions thus lead to a chaotic behavior.

In the following, we investigate whether this chaotic dynamics can be responsible for the irreversibility observed in periodically sheared suspensions. We performed simulations applying a periodic shear with strain amplitudes γ_0 between 0.5 and 6 and a total accumulated strain of 400. The particle mean square displacements are evaluated from the particle positions at the end of each cycle of shear. Changes in the mean-square displacements indicate the presence of irreversible dynamics, whereas the lack of a change in the mean-square displacements from cycle-to-cycle indicate that the system is in a reversible state.

The mean-square displacements obtained in the “pure lubrication limit” do not show, at the particle scale, any significant growth: the system behaves in a reversible way (cf. Fig. 4). This seems at first inconsistent with the chaotic nature of lubrication interactions shown above. However, considering a strain amplitude of $\gamma_0 = 3$, the amplification of perturbations caused by chaos is $e^{\lambda\gamma_0} \approx 5$. The amplification of the noise present in our system [typically round-off error $O(10^{-8})$] is, thus, too small to produce an irreversible displacement observable at the particle scale $O(1)$. Therefore, the chaos arising from lubrication is not responsible for the irreversibility observed in periodically sheared suspensions.

In the “pure contact limit,” the mean-square displacements increase rapidly and then plateau after an accumulated strain $\gamma \approx 150$. The system freezes into a reversible state even at large strain amplitudes. This evolution occurs since the particles driven solely by contact forces organize into layers [see inset of Fig. 4(a)], a configuration in which collisions between particles cease.

A steady fluctuating state is attained at large strain amplitudes when both contact and lubrication interactions are included in the calculations. The lubrication interactions disrupt the formation of layers [see inset of Fig. 4(a)] and consequently particles remain on streamlines where collisions occur. We found that the slope of the mean-square displacement strongly depends on the particle roughness ϵ_r [shown on Fig. 4(a)] but weakly depends on the upper bound of the lubrication range. Note that the above dynamics (self-organization into layers when particles are solely interacting through contacts and the

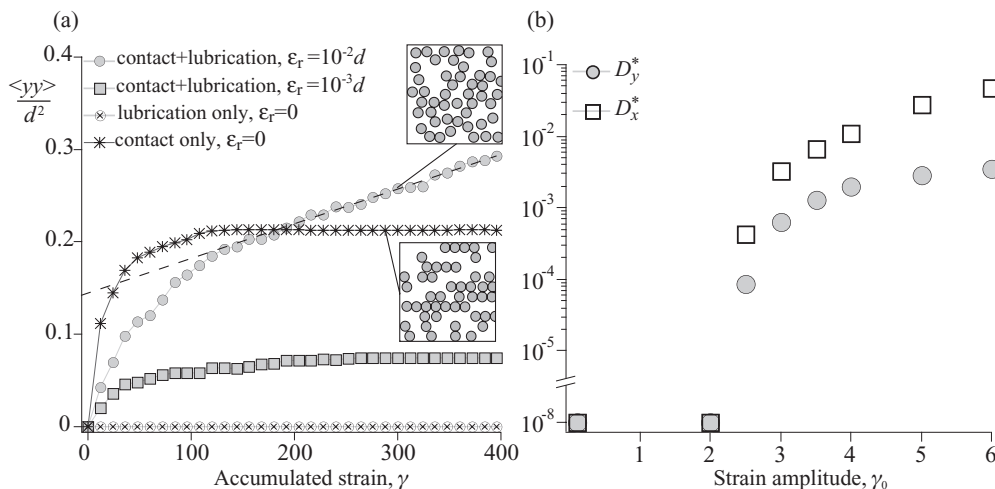


FIG. 4. (a) Mean square displacements versus accumulated strain for $\phi = 0.4$ and $\gamma_0 = 3$. (b) Diffusion coefficients versus strain amplitude for simulations with contact and lubrication interactions for $\phi = 0.5$ and $\epsilon_r = 0.002d$.

disruption of particle layering when lubrication is included) are also observed when simulations are performed with $N = 200$ particles. This suggests that the results are not due to finite-size effects.

The slopes of the particle mean-square displacements for strains of $\gamma > 100$ are used in calculating the dimensionless diffusivities, $D_x^* = \langle xx \rangle / 2\gamma d^2$ and $D_y^* = \langle yy \rangle / 2\gamma d^2$, plotted in Fig. 4(b). The diffusion coefficients parallel, D_x^* , and perpendicular, D_y^* , to the flow direction rapidly increase with strain amplitude. These numerical results agree qualitatively with the experimental data of Pine *et al.* [2] and successfully predict the transition of the particle dispersion at $\gamma_0 \approx 2$. For strain amplitudes smaller than 2, the system self-organizes into a nonfluctuating quiescent state as suggested by the experiments of Corté *et al.* [17].

IV. CONCLUSIONS

We have examined the role of lubrication interactions in suspensions of non-Brownian particles submitted to a periodic shear-flow. We used a simple model that includes repulsive

forces (to prevent overlap) and lubrication (to describe the interaction between particles). We found that chaos arises from the N -body dynamics occurring through the lubrication interactions. However, for the strain amplitudes considered here, $\gamma_0 = [0.25-6]$, this chaos is too weak to produce a significant irreversibility under oscillatory shear. Therefore, in periodically sheared suspensions, lubrication is not responsible for the irreversibility, which is dominated by contact interactions. Nonetheless, lubrication plays an important role by disrupting the particle layering that occurs if particles solely interact through contact forces. Lubrication thus ensures that the collision process perpetuates and allows the system to reach the steady fluctuating state observed in experiments at large strain amplitudes.

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