Bulk and Interface Dispersion of Suspensions in the Inertial Regime

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Hydrodynamic dispersion, i.e., a single particle mean square displacement growing linear in time, occurs in settling non-Brownian mono-disperse suspensions. We use a novel two-dimensional simulation technique for disk-shaped particles settling in a fluid at particle Reynolds numbers up to about Re = 20 to study hydrodynamic dispersion in the bulk suspension and in the sedimentation front separating the suspension from the clear liquid above. In order to analyze the interface broadening due to the particle dispersion we solve a nonlinear convection-diffusion equation for its time evolution. We find that the bulk dispersion coefficients do not fully explain the front evolution, so that either particle-size effects or gradient dependence of the dispersion must be invoked.

1 Introduction

A typical many-particle effect occurring in suspensions is the hydrodynamic dispersion of particles1,2,3,4 i.e., an effectively diffusive long-time behavior of the single-particle displacement, caused by the complex nature of the long-range hydrodynamic interactions. Already the case of three single particles leads to chaotic behavior5 and several experimental and theoretical studies confirm the phenomenon even in mono-disperse viscous suspensions5,7.

Whereas the phenomenon has received much attention for Reynolds number Re → 0, much less is known in the inertial regime Re > 1 which poses tremendous problems to analytical treatment. However, lately, some dynamical simulation techniques for the regime of moderate Re have been developed which allow to study the behavior of suspensions on the level of single particles. These simulation techniques determine the forces on the particles by integration of the surface stresses which are obtained via a finite-difference5,9,10 finite-element,11 or lattice-Boltzmann12 treatment of the liquid subject to no-slip boundary conditions on the container walls and particle surfaces. The particle trajectories follow from integration of the equations of motion. Please see10,9 for the details of the technique employed here.

2 Simulation results

Let us consider a vessel containing a well-stirred homogeneous, mono-disperse suspension settling in negative z direction under the influence of gravity. At the top a relatively well-defined interface separates the bulk suspension from the clear fluid above. During settling the concentration of the suspension remains homogeneous and equals its initial value.

2.1 Hindered settling

Both the bulk particles and the interface settle with the same concentration-dependent velocity \( v_z(\phi) \) which, in three dimensions, is well-described by the phenomenological
Richardson-Zaki relation

\[ v_s^* \equiv v_s(\phi)/v_s = (1 - \phi)^p, \]  

(1)

where \( v_s \) is the terminal velocity of a single particle, \( p \approx 5 \), and \( \phi \) the volume fraction, or in our case area fraction of the suspension. We use asterisks here and in the rest of the text to denote associated dimensionless quantities. In two dimensions we have measured \( v_s^* \) (see Fig. 1a) and find that a value of \( p \approx 3 \) well reproduces our data for particle Reynolds number \( Re = 2av_s/\nu \approx 1 \), where \( a \) is the particle radius and \( \nu \) the clear fluid viscosity. The simulated system’s width is \( 36a \), its height \( 72a \) and it involves about 200 particles at \( \phi = 0.25 \).

2.2 Bulk dispersion

By following the trajectories of single particles and recording the average mean square displacements \( x^2(t) \) after subtracting out the motion of the center of mass we find the hydrodynamic dispersion coefficients. In a finite container we see ballistic behavior of the displacement for short times \( x^2(t) \sim t^2 \), diffusive behavior for intermediate times \( x^2(t) \sim t \), and saturation \( x^2(t) \approx const \), once the particles experience the container constraints. From the behavior at intermediate times \( x^2(t) = (1/2)D_\perp t \) and \( x^2(t) = (1/2)D_\parallel t \) we determine the different dispersion constants \( D_\parallel \) parallel and \( D_\perp \) perpendicular to the direction of gravity. In Fig. 1b we show both \( D_\perp^* \) and \( D_\parallel^* \) with \( D^* = D/(av_s) \) as a function of the area fraction of the systems studied. Each data point has been averaged over 10 dynamical simulations of the settling process.
At very small concentrations hydrodynamic dispersion is small but then rapidly increases as the hydrodynamic interactions between particles increase due to their larger density. A maximum is reached before the dispersion slowly decreases again. Most striking is the high degree of anisotropy because gravity singles out the $z$ direction. At larger volume fraction, where particle collisions and the cage effect start to restrict the motion, the dispersion becomes smaller and more isotropic.

2.3 Temporal evolution of the top interface

Hindered settling and particle dispersion also control the temporal evolution of the interface\textsuperscript{13,14}. There will be (i) a dispersive particle current perpendicular to the front counteracted by (ii) a gravity-induced downward flux of particles. For the first contribution we may assume in analogy with regular diffusion a flux $j_z^*$ opposite to the concentration gradient,

$$j_z^* = -D^*_\parallel(\phi) \frac{\partial}{\partial z^*} \phi.$$  

(2)

Here we have assumed that the dispersion coefficient in the interface equals that of the bulk, although $D^*_\parallel(\phi)$ may well exhibit dependence, e.g., on scalar terms involving the concentration gradient.

To obtain the sedimentation current we multiply the sedimentation velocity with the area fraction of particles. Of course, its sign is negative because the settling is in $-z$ direction.

We then sum these two contributions and express particle conservation using the continuity equation,

$$\frac{\partial \phi}{\partial t^*} + \frac{\partial}{\partial z^*} \left(-D^*_\parallel(\phi) \frac{\partial}{\partial z^*} \phi - \phi v_z^*(\phi)\right) = 0.$$  

(3)

The asterisks indicate dimensionless quantities; all units are in terms of $v_s$ and $a$. This nonlinear equation can be solved analytically only for very specific functional dependence of $D^*_\parallel$ and $v_z^*$ on $\phi$. Here, we solve (3) numerically with a step function as initial condition. The decreasing Richardson-Zaki law (1) leads to self-sharpening of the diffusion front. As models for the diffusive behavior we have employed (i) constant $D^*_\parallel = 0.5$ and (ii) strongly concentration dependent dispersions as $D^*_\parallel(\phi) = 2.5 \exp(-\phi/0.15)$.

In Fig. 2 we show the result of our calculation. On the ordinate we plot the distance from the bottom of the vessel and on the abscissa the concentration $\phi(z^*, t^*)$ as a function of height and time. Points denote simulation values and lines the solutions to Eq. (3) at four consecutive instants. The front moves from the right to the left as it broadens. Surprisingly, the interface is best represented by a model with constant dispersion (i) (dashed lines), whereas several models of type (ii) with very enhanced low concentration dispersion lead to a broad pronounced tail in the dilute region which has no equivalent in the behavior of the simulated interface. As reference, we also plot the solution for the exponential form $D^*_\parallel(\phi) = 2.5 \exp(-\phi/0.15)$ (solid lines). We have varied the functional form of $D^*_\parallel(\phi)$ including forms that start at out at $D^*_\parallel(0) = 0$ and assume a maximum at low concentrations and have
found that the main reason for this tail is that $D_1^a(\phi)$ is significantly larger at concentrations below the bulk value $\phi = 0.25$.

A possible explanation of the deviations is that in our case the front width is too narrow to justify the continuum description (3) and that the discrete particle structure must be taken into account. Another possibility is that the hydrodynamic dispersion constant is sensitive to some scalar expression involving concentration gradients or other higher order fluctuations.

3 Conclusion

Using a novel simulation method we have studied interface and bulk dispersion coefficients in two-dimensional batch settling suspensions in the inertial regime. For a rather concentrated suspension with $\phi = 0.25$ we find that the interface dispersion seems to be smaller than to be expected by the bulk suspension behavior. In particular, the strong asymmetry of the interface profile which is expected from the maximum of the bulk dispersion coefficient at small particle fractions is not seen in the simulation. This observation indicates that either the particulate nature of the problem is important or that we oversimplify the problem by the assumption of an exclusively concentration-dependent dispersion coefficient. We intend to extend our simulation method to three dimensions to be able to directly compare with
experimental results\textsuperscript{13,14} where so far no concentration dependence of \(D^+_\parallel(\phi)\) has been taken into account.

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References