Effects of Container Walls on the Velocity Fluctuations of Sedimenting Spheres

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Simulations describing the settling of suspensions of solid particles bounded by a rigid container are presented. Results are compared with previous simulations of homogeneous suspensions with periodic boundary conditions. Velocity fluctuations in vertically *inhomogeneous* suspensions are found to saturate under conditions similar to those found in laboratory experiments, while in vertically *homogeneous* suspensions, with or without side walls, the velocity fluctuations diverge. A mechanism for the establishment of a correlation length in sedimenting suspensions is proposed.

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In a sedimenting suspension, spatial and temporal variations in particle concentration drive large fluctuations in the particle velocities, of the same order of magnitude as the mean sedimentation velocity. For particles larger than about 10 μm, this hydrodynamic diffusion dominates the thermal Brownian motion, and in the absence of inertia (i.e., at Reynolds numbers close to zero), the particle velocities are determined solely by the instantaneous particle positions. If the particles are randomly distributed, then the velocity fluctuations will diverge with increasing container size [1], although the density fluctuations may eventually drain out of the system by convection [2]. However, experimental measurements indicate that the velocity fluctuations converge to a finite value as the container dimensions are increased [3,4], but the mechanism by which the velocity fluctuations saturate is not yet clear. Koch and Shaqfeh suggested that the distribution of pairs of particles could be modified by shearing forces induced by the motion of a third particle, and that these changes in microstructure could in turn lead to a screening of the long-range hydrodynamic interactions driving the velocity fluctuations [5]. However, detailed numerical simulations found no evidence of the predicted microstructural changes [6]. Instead the velocity fluctuations in homogeneous suspensions (with periodic boundary conditions) were found to diverge with increasing cell size. Recently, it has been proposed that long wavelength density fluctuations can be suppressed by a convection diffusion mechanism [7,8], but a bulk screening mechanism cannot be reconciled with the results of computer simulations [6,9]. Alternatively, it has been suggested that the vertical walls of the container may modify, although not eliminate, the divergence of the velocity fluctuations [10]. Most recently, it has been shown [11] that a small vertical density gradient can damp out diverging velocity fluctuations. We have used numerical simulations to test these theoretical ideas, by comparing the behavior of the velocity fluctuations in three different geometries. We report results of new computer simulations, which use similar geometries to those used in laboratory experiments [3,4], namely a rigid container bounded in all three directions. We find that in this case the calculated velocity fluctuations saturate with increasing container dimensions, as observed experimentally, but contrary to earlier simulations with periodic boundary conditions [6,9]. Moreover, simulations with vertical walls but with periodic boundary conditions at the top and bottom also exhibit diverging velocity fluctuations. Thus we conclude that upper and lower boundaries act as sinks for the fluctuation energy [2], while in homogeneous suspensions velocity fluctuations are proportional to the system size [1]. A scaling argument is used to explain the experimentally observed dependence of the correlation length on volume fraction [4,12].

The simulations reported here used cells with a constant height of $480a$ and square cross sections from $8a$ to $48a$ in width, where a is the particle radius. The largest cell is comparable in width to the smallest cell used in the experiments described in Ref. [3], and about one-half the height. Although larger cells are technically feasible, the present limits are sufficient for the purposes of this study and allow a range of geometries to be conveniently studied. The particle volume fraction was set at $\phi = 13\%$, so that the mean interparticle spacing $a\phi^{-1/3}$ is almost exactly $2a$. The simulations contained between 1000 and 35 000 solid particles, and were bounded in the horizontal (xy) plane by vertical no-slip walls. In one set of calculations the container was also bounded at the top and bottom by no-slip walls, whereas in the other set of calculations periodic boundary conditions were used in the vertical (z) direction. In the vertically bounded suspensions, the chosen container height gave a maximum sedimentation time of about $600t_s$, where $t_s = a/U_0$ is the Stokes time and U_0 is the velocity of an isolated particle. Simulations with periodic boundary conditions in the vertical direction use an imposed pressure gradient to generate an upcurrent of fluid and maintain a steady force on the particle phase, balancing the gravitational field. These new results are compared with previous simulations using periodic boundary conditions in all directions [6,9].

The numerical simulations are based on a lattice-Boltzmann model of the fluid phase [13,14], with modifications and improvements that will be described in more

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detail elsewhere. The Reynolds number based on the mean sedimentation velocity $\langle U_z \rangle$, $\mathrm{Re} = 2\langle U_z \rangle a/\nu = 0.2$, was chosen for computational efficiency, and is 2–3 orders of magnitude larger than in laboratory experiments. However, additional simulations (see Table I) indicate that reductions in Reynolds number have only a small effect on the velocity fluctuations. The particle radius, $a = 1.25$ lattice spacings, was also chosen to minimize the computational cost, but is sufficient for the purposes of this paper. This is because velocity fluctuations in low-density suspensions are dominated by long-range hydrodynamic interactions, which are correctly reproduced even by small particles. In addition, the simulation method described in Refs. [13,14] has been improved by incorporating the exact lubrication forces between pairs of spheres and between spheres and plane walls. The largest simulations contain about 2×10^6 fluid nodes and 35 000 solid particles. A run of 600 Stokes times requires 75 000 time steps, or about 200 hours of CPU time on a 600 MHz Pentium PIII processor.

The mean-square fluctuations in particle velocity, averaged over the cross-sectional area of the container, have been determined as a function of the container width. Our calculations of the vertical velocity fluctuations, $\langle \Delta U_z^2 \rangle$, take into account the variation in mean sedimentation velocity across the cell, although this is not a qualitatively important issue. Averages over the whole cell (as measured in Ref. [4] and used in Fig. 1) are 10–20% smaller than those measured in the middle of the cell. In vertically homogeneous suspensions, fluctuations were also averaged over the height of the periodic unit cell, whereas for vertically bounded suspensions, the fluctuations were averaged over a window of height $160a$ (one-third of the container height), centered one-third of the way up the container. This viewing window is clear of both the sediment layer at the bottom of the vessel and the location of the sedimentation front at the end of the simulation. It is unclear whether or not the system reaches a steady state before the sedimentation front reaches the top of the viewing window (see Fig. 2). A similar issue may be encountered in laboratory experiments as well [12]. To minimize the possible effects of the lack of a steady state, we use the same time window for all these simulations, namely from 300 to 600 Stokes times. Vertically homogeneous suspensions were averaged over a steady state of similar duration (400 Stokes times), but the increased volume available for measurements reduces the statistical errors by a factor of 2, to less than 5%.

The main result of this paper is illustrated in Fig. 1, and shows that the velocity fluctuations in a bounded container are independent of container width for sufficiently large containers. On the other hand, in vertically homogeneous suspensions velocity fluctuations are proportional to the container width, regardless of the boundary conditions in

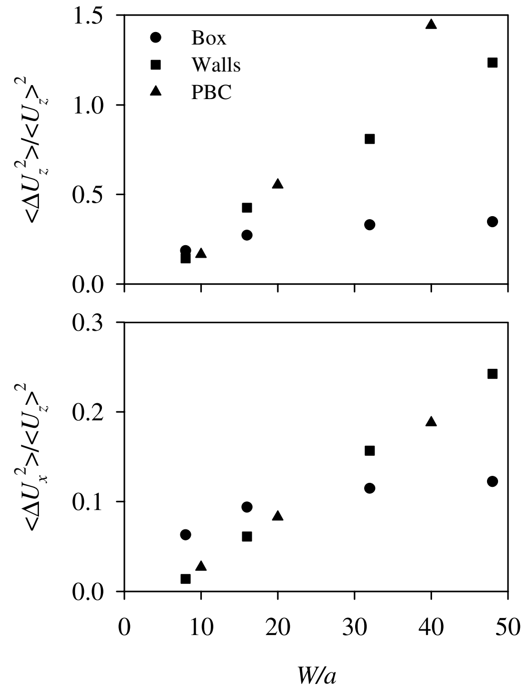

FIG. 1. Relative velocity fluctuations $\langle \Delta U_\alpha^2 \rangle / \langle U_z \rangle^2$ as a function of container width. The vertical ($\langle \Delta U_z^2 \rangle$) and horizontal ($\langle \Delta U_x^2 \rangle$) fluctuations are shown for three different boundary conditions: a cell bounded in all three directions by no-slip walls (box), a cell bounded by vertical walls (walls), and a cell that is periodic in all three directions (PBC) [6,9]. The statistical errors are comparable to the size of the symbols.

TABLE I. Variation in velocity fluctuations with Reynolds number and particle radius. These simulations used a system of 3840 particles and the velocity fluctuations were averaged over a time window $300t_s < t < 600t_s$.

a	Re	$\langle \Delta U_z^2 \rangle / \langle U_z \rangle^2$	$\langle \Delta U_x^2 \rangle / \langle U_z \rangle^2$
1.25	0.20	0.21	0.077
1.25	0.10	0.19	0.070
1.25	0.05	0.20	0.079
1.25	0.02	0.19	0.077
2.70	0.20	0.27	0.059

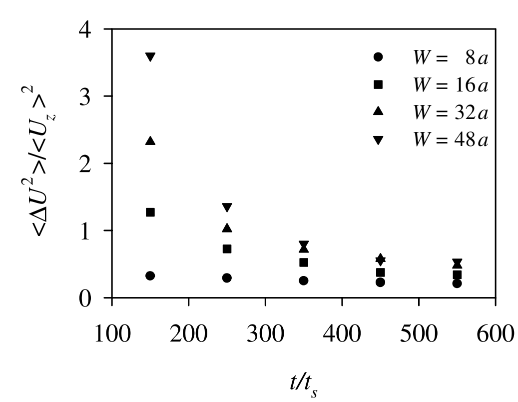

FIG. 2. Time dependence of the relative velocity fluctuations, $\langle \Delta U^2 \rangle / \langle U_z \rangle^2$, for four different container widths.

the horizontal plane. The significance of this result is that it establishes unambiguously that velocity fluctuations in a sedimenting suspension do depend on the macroscopic boundary conditions and that laboratory measurements [3,4,12] are not characteristic of a uniform suspension, as has been supposed. Instead, the simulations show that vertical variations in particle concentration are responsible for suppressing the velocity fluctuations, which otherwise diverge with increasing container size, in agreement with theory [1] and earlier simulations [6,9]. We conclude that attempts to explain the experimental observations by invoking a bulk screening of the hydrodynamic interactions [5,7,8] are incorrect.

The simulations also show that vertical walls do not play a qualitatively important role in determining the magnitude of the velocity fluctuations. The horizontal velocity fluctuations are quantitatively similar for suspensions with periodic boundary conditions in the horizontal plane and suspensions bounded by vertical walls. Nevertheless, the side walls reduce the amplitude of the vertical fluctuations, without altering the dependence on container width, thereby reducing the anisotropy, $\langle \Delta U_z^2 \rangle : \langle \Delta U_x^2 \rangle$, from about 7:1 to about 5:1, which is close to the experimental measurement of 4:1. Vertical walls may play an important role in determining the fluctuations in thin cells [10], but our results show that they do not suppress the divergence observed in vertically homogeneous suspensions.

In vertically homogeneous suspensions, the amplitude of the velocity fluctuations rapidly approaches a steady state, on a time scale of the order of 100 Stokes times. However, when the container is bounded at the bottom by a rigid wall the fluctuations decay slowly in time, as shown in Fig. 2. The maximum in the fluctuation energy, $\langle \Delta U^2 \rangle = \langle \Delta U_z^2 \rangle + 2\langle \Delta U_x^2 \rangle$, is comparable to the steady-state values in homogeneous suspensions, but at long times ($t > 300t_s$), the velocity fluctuations, measured over the same vertical window, are independent of container size for sufficiently large vessels. These new simulations suggest that the container bottom and the suspension-supernatant interface act as sinks of fluctuation energy, as suggested earlier by Hinch [2]. Random density fluctuations convect to one of these two interfaces and are absorbed by the density gradient at the interface. Scaling arguments suggest that a horizontal density fluctuation of length l convects with a velocity $v_l \approx U_0\sqrt{\phi l/a}$ [2], so that fluctuations drain away on a time scale $t_C(l) \approx l/v_l \approx \sqrt{l/a\phi}\, t_s$. Although the present simulations do not unambiguously evolve to a steady state before the sediment front reaches the viewing window, experimental results with taller vessels [3,4] do show a regime where the velocity fluctuations are time independent. If we assume that density fluctuations are generated at small scales [8] (of order a) by conversion of gravitational potential energy, and spread out by diffusion, then they will grow to a length scale l in a time of order $t_D(l) \approx l^2/D$, where $D \approx U_0 a$ is the hydrodynamic dispersion coefficient. By balancing the convection time t_C with the diffusion time t_D we obtain a critical length scale, $l_c \approx a\phi^{-1/3}$, beyond which fluctuations drain away more rapidly than they can be replenished by diffusion. Thus the system can reach a steady state with a correlation length that is independent of system width and proportional to the mean interparticle spacing $a\phi^{-1/3}$, as observed experimentally [4,12]. This picture suggests that the time to reach steady state will depend on the height of the container; calculations are in progress to test this hypothesis.

It has recently been proposed that a vertical concentration gradient could develop in a suspension bounded by a bottom wall [11], and that density fluctuations would then convect to their position of mechanical equilibrium, rather than decaying by diffusion or by drainage to the upper and lower boundaries. It has been shown that in this case the velocity fluctuations are bounded and decay as $t^{-1/2}$ [11], which is qualitatively consistent with the data shown in Fig. 2. However, we have not been able to confirm the presence of a vertical concentration gradient in the suspension, since it is obscured by the statistical fluctuations in particle density. The data shown in Fig. 3 suggest that $l \approx 10^4 a$, although at this point even the existence of a density gradient is uncertain. In the future we plan to examine a steady-state, fluidized bed, which will allow for extensive time averaging and a better determination of l.

The simulations described in this paper are not expected to be a completely quantitative description of Stokes-flow hydrodynamics. In particular, we cannot disregard the possibility that inertial effects play a role on scales larger than the particle radius. At the volume fraction used in this work, we can expect that particle velocity correlations persist for distances of the order of $50a$ [4], and the Reynolds number based on this distance is of the order of 5. However, the striking dependence of the velocity fluctuations on the macroscopic boundary conditions makes it unlikely that our qualitative conclusions will be affected by more

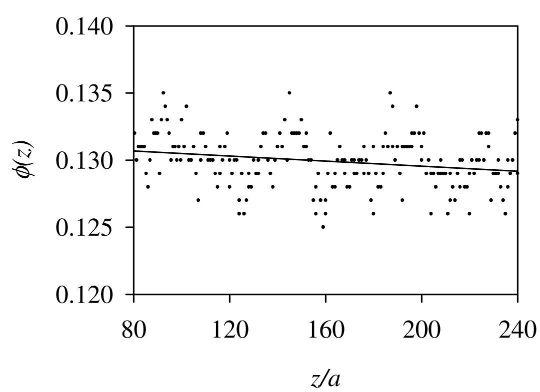

FIG. 3. Particle volume fraction as a function of height. The particle density in the viewing window ($80a < z < 240a$) was averaged over the last 200 Stokes times of the simulation ($400t_s < t < 600t_s$). A least-squares fit (solid line) gives a slope of about 10^{-5}, corresponding to $l \approx 13000a$.

accurate simulations. Nevertheless, additional simulations have been made to assess the effects of the approximations made in these calculations on the velocity fluctuations. The calculations are limited to a system bounded in all three directions, with a width of $16a$ and containing 3480 particles. The data in Table I show that for Reynolds numbers in the range $0.02 < \mathrm{Re} < 0.2$ there is no systematic effect on the velocity fluctuations, which are all within the 10% statistical errors of the simulations. We do see a statistically significant variation in the velocity fluctuations with particle size. The total fluctuation energy $\langle \Delta U^2 \rangle$ is not affected, but the anisotropy of the fluctuations is larger, and closer to the experimental measurements. Based on previous calculations [9], we do not expect that simulations with even larger particles would be significantly different from the results with $a = 2.7$. From the data in Table I we conclude that the calculations reported here are free of qualitatively significant numerical errors.

In this work we have shown that horizontal walls affect the amplitude and system-size dependence of the velocity fluctuations in a sedimenting suspension. In vertically homogenous suspensions the fluctuations are limited by the horizontal container dimensions, whereas the imposition of a no-slip boundary condition at the base of the container causes the fluctuations to saturate at a much smaller value, independent of the container width. These new simulations support the conclusions of earlier theoretical [1] and numerical [6] studies, which found that the velocity fluctuations in a homogeneous suspension are proportional to the container size. The contradictory experimental findings [3,4] have now been shown to arise from inhomogeneities induced by the container base. We have proposed an explanation of the experimental observations based on an extension to the model proposed by Hinch [2], which leads to a time-independent correlation length proportional to the mean interparticle spacing and independent of system size. Our results contradict the notion [5,7,8] that there is a bulk screening mechanism operating in homogeneous suspensions.

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