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Shear-induced particle diffusion in inelastic hard sphere fluids

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A large-scale numerical simulation of a system of inelastic, rough, hard spheres of volume fraction $\phi_S = 0.565$, starting from a disordered configuration in a Couette geometry, shows a transition to a layered state, which possesses long-range orientation order, after long run times. This phase transition is shown to cause a dramatic decay of the long-time transverse self-diffusion coefficient of particles. As the solid volume fraction is increased to 0.58, the dimensionless transverse self-diffusion coefficient decays further, approaching a value of order 10^{-5}, which indicates structural arrest. [S1063-651X(98)50811-2]

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In a sheared granular flow, grains do not move along streamlines but instead exhibit fluctuating motions due to encounters with their neighboring grains. Hence, the grains within the assembly are continually losing information concerning their relative positions due to shearing. This loss of information characterizes the diffusive motion of the grains. Recently, computer simulations have been used to develop a better understanding of diffusion processes in unbounded dense granular shear flows [1]. This attempt led to a conjecture that a rapidly flowing monosized granular material is a diffusive system except at large solids concentrations. It was reported that at a volume fraction $\phi_c \approx 0.56$, the grains appeared to be trapped in a microstructure and prohibited from moving relative to their neighbors. This behavior, which characterizes a crystalline system, has not been observed in experiments of rapid granular flows between parallel rough boundaries [2]. In contrast, clear experiment evidence [2] exists for the movement of the particles in directions transverse to the bulk motion at even higher solid concentrations than those examined in the previous simulations [1].

Diffusion processes are of considerable importance in dense granular flows occurring in common industrial systems, for which the significance of interactions between the grains and the boundaries on the flow dynamics is obvious. Hence, it is important to examine whether a transition volume fraction, ϕ_c, exists for a confined dense granular flow of monosized particles. To this end, three-dimensional computer simulations of the flow of a system of dense, rough, inelastic, optically bidisperse hard spheres, with 4296 interior particles that are the same in terms of size and interaction, but have different colors, are carried out in a Couette geometry. Since a color label plays no role in the particle dynamics, the algorithm presented in a previous study [3] can be used to create the particles trajectories in a rectangular periodic computational box (with the lengths of the three sides of the box equal to $L_x = 1$, $L_y = 1$, and $L_z = 0.497$). The reader is referred there for more details, including a geometrical description of the problem. The walls are comprised of 400 hemispherical massive particles (with the same diameter as the interior particles) positioned at $Z = \pm L_z/2$, and no periodic boundary conditions are assumed in the directions normal to the walls.

In contrast to the previous simulations [1] in which the particles were initially organized in a triangular prismatic packing, the initial disordered hard-sphere configuration is created using the technique described by Clarke and Wiley [4]. For the present simulations, an initial set of random overlapping spheres is chosen. Then the individual spheres are moved randomly until the overlaps are removed. On one side of the labeling plane, $Z = 0$, the particles are dark in color, whereas on the other side the particles are light in color. The snapshot of the initial configuration of dark colored particles, projected onto the plane normal to the shear flow in the x direction (which is the yz plane in this work), is shown in Fig. 1(a).

A shear flow is applied to the aforementioned system of hard-dissipative spheres, by increasing average shear rate from zero to $\gamma = 2U/L_z \approx 4\ \mathrm{s}^{-1}$. Here U represents the velocity of one of the walls. Dissipation induced by particle-particle collisions is modeled using a coefficient of restitution, $e = 0.84$, as well as a surface friction coefficient, $\mu = 0.41$ [5]. The values of the dissipation parameters are chosen to be close to those used in the previous simulations [1].

For sufficiently long run times, the system eventually reaches an equilibration state in which the amount of energy supplied by shearing is balanced by that lost due to dissipative collisions as well as frictional interactions. In order to monitor the evolution of the system toward a state of equilibration, the instantaneous values of dimensionless normal stress exerted by the particles on the bottom wall [6] are recorded. The manner in which the dimensionless normal stress, P^*, of the aforementioned system varies with dimensionless time, $t^* = tU/L_z$, is illustrated in Fig. 2. The decay of the absolute value of mean dimensionless normal stress, $|\overline{P^*}|$, appears to be almost exponential for $t^* < 200$. There is, however, a significant decrease of $|\overline{P^*}|$ at about $t^* \approx 200$, which is clear evidence of a phase transition.

