Shear induced diffusive mixing in simulations of dense Couette flow of rough, inelastic hard spheres

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Large-scale numerical simulations of a system of inelastic, rough, hard spheres of volume fraction \( \phi_s = 0.565 \), which are initially distributed randomly in a Couette geometry, show clear evidence of the movement of the particles in directions transverse to the bulk motion. This behavior of the aforementioned system, which has been considered as a model for a granular fluid, is consistent with recent experimental observations [Hsiau and Hunt, J. Fluid Mech. 251, 299 (1993)]. Based on the results obtained, there are indications that a bounded rapid granular flow could be a diffusive system at volume fractions even higher than 0.56. This finding contradicts earlier computer experiments [Campbell, J. Fluid Mech. 348, 85 (1997)] which found a rapidly flowing granular material is a diffusive system except at large solids concentrations (i.e., \( \phi_s > 0.56 \)). © 1998 American Institute of Physics. 

Recently, attention has been devoted to the role of inelastic collisions in granular hydrodynamics.\(^1\)\(^2\) Using stainless steel particles with a low coefficient of friction, in a two-dimensional system of spherical particles, Kudrolli, Wolpert, and Gollub\(^1\) have observed the formation of clusters at high particle densities. Moreover, in a computer experiment of a moderately dense three-dimensional Couette flow of hard, smooth, dissipative spherical particles of uniform size, stringlike clusters were produced.\(^2\) The presence of stringlike clusters in the aforementioned system below the freezing-point volume fraction of hard-sphere fluids\(^3\) (i.e., \( \phi_s = 0.494 \)), indicates the importance of inelastic collisions which could lead to cluster formation. It is expected, however, that with increasing particle volume fraction, a fluid composed of hard dissipative spherical particles exhibits a soliddlike order under shear.\(^4\) This behavior plays a crucial role in calculating transport properties of a system such as a dense granular fluid for which the interparticle interactions may be assumed to be close to those of hard dissipative spheres. The estimation of the contribution of various correlated or non-Markovian events is of interest in dense granular fluids where long-time interactions of the particles may become significant.

In order to indicate what important effects should be considered in developing a theory for rapid granular flows, Campbell\(^5\) has reported measurements of the particle diffusive motion in an unbounded dense granular shear flow using computer simulations. Unexpectedly, at the solid volume fraction of \( \phi_s = 0.56 \), the particles appeared to be trapped in a microstructure and prohibited from moving relative to their neighbors, which indicates a transition to a stable ordered state. Campbell conjectured that a rapidly flowing granular material is a diffusive system except at large solid concentrations. However, there is clear experimental evidence\(^6\) for the movement of the particles in directions transverse to the bulk motion at even higher solid concentrations than those examined in Campbell’s simulations. Clearly, further investigation is required to determine the reasons for the apparent discrepancy between the simulations and the experiments.

The motivation for this work is to investigate whether diffusive mixing occurs in bounded rapid shear flows of a system of dense, rough, inelastic hard spheres at volume fractions higher than 0.56. Numerical simulations are the most convenient technique available to study diffusive mixing in a sheared, dense, hard-dissipative-sphere fluid approaching a thermal equilibrium state\(^7\) from an initial nonequilibrium disordered state. In fact, at high volume fractions, thermal equilibrium in a hard-dissipative-spheres system is metastable,\(^8\) and therefore, shearing may cause crystallization, which ultimately results in the vanishing of diffusive mixing.

In order to obtain an overview of particle diffusive mo-