

Hydrodynamics of fluid-solid coexistence in dense shear granular flow

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(Received 25 September 2006; published 31 May 2007)

We consider dense rapid shear flow of inelastically colliding hard disks. Navier-Stokes granular hydrodynamics is applied accounting for the recent finding that shear viscosity diverges at a lower density than the rest of the constitutive relations. New interpolation formulas for constitutive relations between dilute and dense cases are proposed and justified in molecular dynamics (MD) simulations. A linear stability analysis of the uniform shear flow is performed and the full phase diagram is presented. It is shown that when the inelasticity of particle collision becomes large enough, the uniform sheared flow gives way to a two-phase flow, where a dense “solidlike” striped cluster is surrounded by two fluid layers. The results of the analysis are verified in event-driven MD simulations, and a good agreement is observed.

DOI: 10.1103/PhysRevE.75.051310

PACS number(s): 45.70.Mg, 45.70.Qj, 83.50.Ax

I. INTRODUCTION

Granular shear flows have attracted much attention in recent years [1]. However, theoretical description of *dense* granular flows still remains a challenge [2]. The present work focuses on a *rapid dense* flow of inelastic hard disks, which undergo a shear motion. Here, the medium is fluidized, particle collisions are binary and instantaneous. This brings about a possibility of a hydrodynamic description of granular media [3].

There are still significant difficulties in the hydrodynamic description of *dense* shear flows, even within the model of inelastic hard spheres. Although for low and moderate densities, a hydrodynamic description with the proper constitutive relations can be derived from kinetic theories [4], constitutive relations for dense flows are presently unknown. Several attempts to extend the theory to high densities have been done recently [5–8]. It was proposed to apply free volume arguments [5,9] in the vicinity of close-packing density, $n_{\max} = 2/(\sqrt{3}d^2)$, and use interpolation functions for constitutive relations between low- and high-density cases [5–8]. At high densities, there is another problem related to the behavior of shear viscosity [8,10,11]. While inelastic heat losses, thermal conductivity, and pressure diverge at the close-packing density n_{\max} , it was shown recently that shear viscosity diverges at a lower density [8]. This may result in the coexistence of fluid and solid phases [11].

We propose here interpolation formulas for constitutive relations between low-density and high-density cases, which account for viscosity divergence, and justify them in molecular dynamics (MD) simulations. We employ the resulting granular hydrodynamics for *quantitative* description of fluid-solid coexistence in shear granular flow and verify the hydrodynamic predictions in MD simulations.

II. THE MODEL AND GOVERNING HYDRODYNAMIC EQUATIONS

Consider a plane Couette geometry: an ensemble of inelastically colliding hard disks with unit masses and diameter d is driven, at zero gravity, by two walls. The top wall, located at $y=H/2$, moves in the x direction with velocity u_0 ,

the bottom wall moves in the opposite direction with the same velocity. The only parameter that characterizes the inelasticity of collisions is the coefficient of normal restitution, r . Boundary conditions in the x direction are periodic. In the y direction, no-flux and no-slip boundary conditions are implemented. Upon a collision with a driving wall, the normal particle velocity switches sign, while the new tangential velocity component is taken from the Maxwell-Boltzmann distribution, with a mean equal to the wall velocity, and a variance corresponding to an instant temperature of the layer next to the wall.

Now we present a hydrodynamic approach, which deals with the number density of grains, $n(\mathbf{r}, t)$, the granular temperature $T(\mathbf{r}, t)$, and the mean flow velocity [4],

$$dn/dt + n \nabla \cdot \mathbf{v} = 0,$$

$$n(d\mathbf{v}/dt) = \nabla \cdot \mathbf{P},$$

$$n(dT/dt) = -\nabla \cdot \mathbf{Q} + \mathbf{P} : \nabla \mathbf{v} - \Gamma, \quad (1)$$

where \mathbf{P} is the stress tensor, \mathbf{Q} is the heat flux, and Γ is the energy loss due to the inelasticity of particle collisions. The stress tensor \mathbf{P} is given by $\mathbf{P} = [-p(n, T) + \mu(n, T)\text{tr}(\mathbf{D})]\mathbf{I} + 2\eta(n, T)\hat{\mathbf{D}}$, where $\mathbf{D} = (1/2)[\nabla \mathbf{v} + (\nabla \mathbf{v})^T]$ is the rate of deformation tensor, $\hat{\mathbf{D}} = \mathbf{D} - \frac{1}{2}\text{tr}(\mathbf{D})\mathbf{I}$ is the deviatoric part of \mathbf{D} , and \mathbf{I} is the identity tensor, $\eta(n, T)$ and $\mu(n, T)$ are the shear (first) and bulk (second) viscosities. The heat flux \mathbf{Q} is given by $\mathbf{Q} = -\kappa(n, T)\nabla T$, where $\kappa(n, T)$ is the coefficient of thermal conductivity. An additional term in the expression for heat flux, proportional to the *density* gradient [12,13], can be neglected in the nearly elastic limit $1-r^2 \ll 1$ we consider throughout this paper. For higher values of inelasticity one also needs to take into account inelastic corrections to transport coefficients [12]. However, the main point of the present paper is addressing the challenging problem of describing a very dense flow and (as the first step) it is sufficient to assume the limit of nearly elastic particle collisions.

III. TESTING CONSTITUTIVE RELATIONS IN MD SIMULATIONS

For dilute and moderately dense granular flows, the Enskog-type constitutive relations are derived from kinetic theory [4]. The shear viscosity, $\eta_E(n, T)$, the thermal conductivity $\kappa_E(n, T)$, the inelastic heat losses $\Gamma_E(n, T)$, and the equation of state p_E are given by

$$\eta_E = \frac{4\nu T^{1/2} G_E}{\pi^{3/2} d} \left[1 + \frac{\pi}{8} \left(1 + \frac{1}{G_E} \right)^2 \right],$$

$$\kappa_E = \frac{8\nu T^{1/2} G_E}{\pi^{3/2} d} \left[1 + \frac{9\pi}{16} \left(1 + \frac{2}{3G_E} \right)^2 \right],$$

$$\Gamma_E = \frac{8(1-r)nT^{3/2}G_E}{\pi^{1/2}d},$$

$$p_E = nT(1 + 2G_E), \quad (2)$$

where $G_E = \nu(1 - 7\nu/16)/(1 - \nu)^2$, $\nu = n(\pi d^2/4)$ is the solid fraction, and index E stays for ‘‘Enskog.’’ For small and moderate densities and for small inelasticities, transport coefficients are in a reasonable agreement with the results of event-driven MD simulations [14]. For very large densities, one can use free volume arguments [5,9] and show that all the constitutive relations (except for shear viscosity) diverge at the density of close packing. However, there is strong evidence that at high densities the coefficient of shear viscosity behaves differently than other constitutive relations [8,10], diverging at a *lower* density than other transport coefficients [8]. An immediate consequence of this finding is a possible existence of a solidlike phase, which is at rest or moves as a whole, as its density is higher than the density of viscosity divergence [11]. Khain and Meerson [11] considered a very dense three-dimensional system and assumed a leading order expansion of constitutive relations (except for shear viscosity) near the close-packing density. However, to employ hydrodynamic equations within a wide range of densities, one needs a pragmatic approach involving interpolation of constitutive relations between the dilute and dense cases [5–8]. We will adapt this approach, suggesting several interpolation functions, and testing them in MD simulations.

To begin with, a global equation of state of hard disk fluid was recently proposed [6,8], $p = nT(1 + 2G)$, where $G = G_E + m[\nu_{\max}/(\nu_{\max} - \nu) - G_E]$. Here, m is an interpolation function, given by $m = \{1 + \exp[(\nu_c - \nu)/m_0]\}^{-1}$ with $\nu_c = 0.70$, $m_0 = 0.0111$, and $\nu_{\max} = \pi/(2\sqrt{3})$, in a good agreement with MD simulations [6]. According to the same lines, we propose the modified form of inelastic heat losses, changing G_E to G in the corresponding expression in Eqs. (2). To test this expression in MD simulations, we consider a completely different system: a homogeneous freely cooling ensemble of inelastic hard disks in a box. In this case the third equation of Eqs. (1) becomes $n\partial T/\partial t = -\Gamma$, which gives the well-known Haff’s law [4], $T = (1 + t/t_0)^{-2}$. Here temperature is measured in units of the initial temperature T_0 , and time in units of $HT_0^{-1/2}$, where H is the system width. In our case, $t_0 = (\pi^{1/2}/4)(d/H)[(1-r)G]^{-1}$. We measured the temperature as

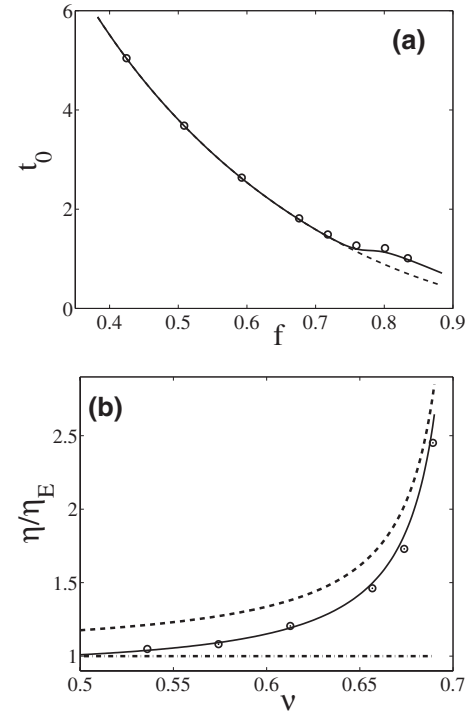


FIG. 1. Testing constitutive relations in MD simulations: heat losses (a) and shear viscosity (b). (a) A time scale for a temperature decay, t_0 , as a function of density both from theory (solid line) and MD simulations (circles). The Enskog predictions (dashed line) do not agree with the results of MD simulations at high densities. The restitution coefficient is $r=0.999$ (the simulation with the highest density was performed for $r=0.9999$ and then the value of t_0 was properly recalculated), the total number of particles is $N=6480$, and the system aspect ratio is $\delta=0.8$. (b) The coefficient of shear viscosity normalized by the Enskog value as a function of density. Enskog formula (dashed-dotted line) disagrees completely with MD simulations (circles) at high densities. Also shown are the expression in Ref. [8] (dashed line) and the new interpolation formula (solid line). The total number of particles is $N \approx 6400$, and the restitution coefficient is very close to unity (ranging from $r=0.996$ to $r=0.99995$ in different MD simulations), to ensure that the solution of uniform shear flow is realized.

a function of time in MD simulations within a wide range of densities, while other parameters were kept constant. To ensure the homogeneous cooling state being stable [15], we took a sufficiently large restitution coefficient. As expected, we found the Haff’s law to be valid and computed the value of t_0 . Figure 1(a) shows t_0 versus $f = \langle \nu \rangle / \nu_{\max}$, both from the theory (solid line) and MD simulations (circles). A good agreement is observed, in contrast to the Enskog predictions (dashed line), which deviate from the results of MD simulations at high densities.

The next step is specifying the coefficient of shear viscosity. Consider a dense uniform shear flow. Here, the energy balance equation reduces to $\eta(du/dy)^2 = \Gamma$. Measuring the temperature of the system in MD simulations at different densities, we calculate the inelastic heat losses, and compute the shear viscosity η . In Ref. [8], the coefficient of shear viscosity of a system of elastic hard disks was measured using the Helfand-Einstein expressions. It was found that η

diverges like $a_\eta(\nu_\eta - \nu)^{-1}$, where the viscosity divergence density is $\nu_\eta = 0.71$, and $a_\eta = 0.037$ [8], in contrast to the Enskog predictions. Our MD simulations confirm this result. Figure 1(b) shows that the Enskog formula (dashed-dotted line) dramatically disagrees with MD simulations (circles) at high densities. An interpolation between dilute and dense regimes was also proposed in Ref. [8], $\eta_L = \eta_E[1 + a_\eta/(\nu_\eta - \nu)]$, see Fig. 1(b), the dashed line. Since this interpolation is not accurate for the intermediate densities, we propose an improved interpolation function $\eta = \eta_E[1 + a_\eta(\nu/\nu_\eta)^3/(\nu_\eta - \nu) - a_\eta/\nu_\eta]$. The new formula (solid line) agrees well with MD simulations in a wide range of densities.

In Ref. [8], the coefficient of thermal conductivity κ was also measured in MD simulations. It was found to be larger than κ_E for intermediate densities ($\nu \approx 0.55$), and smaller than κ_E for larger densities, $\nu \approx 0.75$ (see Fig. 7 in Ref. [8]). Thermal conductivity is known to diverge at the close-packing density, as $(\nu_{\max} - \nu)^{-1}$. Incorporating these findings, we propose the following interpolation formula: $\kappa = \kappa_E[1 + 0.1\nu - 10\nu^{10} + 0.11(\nu_{\max} - \nu)^{-1} - 0.11/\nu_{\max}]$, which is in a good agreement with the results of Ref. [8]. Now, we apply the resulting granular hydrodynamics to the problem of dense shear flow.

IV. STEADY DENSE SHEAR FLOW: MD SIMULATIONS VERSUS HYDRODYNAMICS

Let us measure the coordinate y in units of the system height H , the horizontal velocity u in units of the wall velocity u_0 , the temperature T in units of u_0^2 , the density n in units of n_{\max} , the pressure P in units of $n_{\max}u_0^2$. Then the steady shear flow ($\partial/\partial t = 0, v = 0, \partial/\partial x = 0$) is described by the following system of equations:

$$\frac{d}{dy} \left(f_2 T^{1/2} \frac{du}{dy} \right) = 0, \quad f_4 T = \text{const},$$

$$\frac{d}{dy} \left(f_1 T^{1/2} \frac{dT}{dy} \right) + \frac{f_2 T^{1/2}}{4} \left(\frac{du}{dy} \right)^2 - R f_3 T^{3/2} = 0, \quad (3)$$

where $R = (16/\pi)(1-r)(H/d)^2$ is the heat loss parameter, and the functions f_i are the density-dependent parts of the constitutive relations, $f_1 = \kappa(\sqrt{\pi}d/2)T^{-1/2}$, $f_2 = \eta(2d\sqrt{\pi})T^{-1/2}$, $f_3 = \nu G$, and $f_4 = n(1+2G)$. No-flux and no-slip boundary conditions are given by $dT/dy(y=-1/2) = dT/dy(y=1/2) = 0$, $u(y=-1/2) = -1$, $u(y=1/2) = 1$. The total number of particles is conserved, which yields a normalization condition for the density, $\int_{-1/2}^{1/2} n(y) dy = f$, where $f = \langle \nu \rangle / \nu_{\max}$ is the average area fraction. Equations (3) allow for different solutions. The simplest one is the uniform shear flow. In this case, density and temperature are constant, and the velocity profile is linear. For low and moderate densities, it is known that uniform shear flow becomes unstable, when the inelasticity of particle collisions exceeds a critical value [16–18]. This problem has been analyzed by linear stability analysis of the corresponding equations of granular hydrodynamics [16–18]. The instability may result in shear-band formation, which was recently observed in MD simulations [19] and analyzed

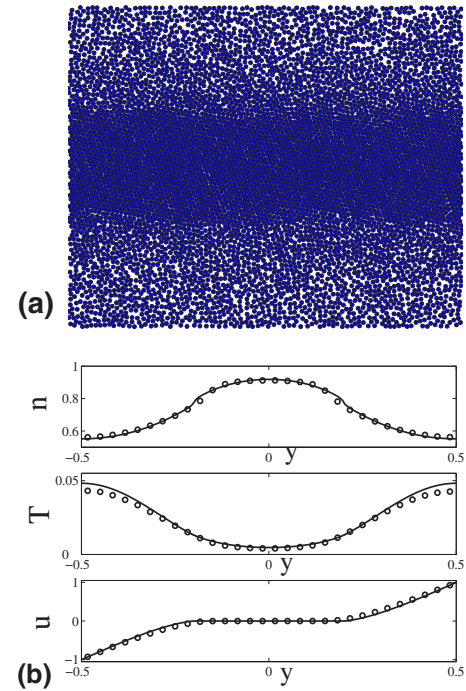


FIG. 2. (Color online) A two-phase solution. (a) A snapshot of the system from MD simulations at $t \approx 9 \times 10^3$. The solidlike layer in the middle (which is at rest) is surrounded by two fluid layers. (b) The corresponding hydrodynamic profiles: theory versus MD simulations. The density (upper panel), temperature (middle panel), and velocity (lower panel) profiles in the system, both from solution of Eqs. (3) (solid lines) and from MD simulations (circles). The total number of particles is $N = 6480$, the restitution coefficient is $r = 0.99$, the system dimensions are $L \approx 97d$, $H \approx 80d$. The corresponding hydrodynamical parameters are $R = 323.86$ and $f = 0.7242$.

theoretically for moderate densities [17], see also [18]. We found that for high densities, the same instability exists, but its threshold changes qualitatively. Indeed, as a result of shear viscosity divergence at $\nu_\eta < \nu_{\max}$, the uniform shear flow solution is impossible at sufficiently large average density, $f > \nu_\eta / \nu_{\max}$. When this solution does not exist or is unstable, the density profile is no more homogeneous. In this case, the regions with the density larger than that of viscosity divergence may appear. Although, those regions are at rest or move as a whole, the granulate is fluidized there and granular temperature is not zero [11].

Our MD simulations show that when R is large enough, the system consists of three layers: an inner solidlike layer and two outer fluid layers, see example of a snapshot in Fig. 2(a). This fluid-solid coexistence has been recently observed in MD simulations [19,20]. To describe it hydrodynamically, one needs to solve Eqs. (3) for each layer separately, demanding continuity of the density, of the heat flux, and of the velocity at the interfaces between the layers. For the solidlike layer, the first equation of Eqs. (3) is replaced by $u = \text{const}$, whose value should be found from the overall solution. We find the solution of Eqs. (3) using a numerical shooting procedure, similar to that described in [11]. Interestingly, there exists a family of solutions (missed in [11]), which can be parametrized by the position of density maximum in the system. In this study we only consider solutions with a symmet-

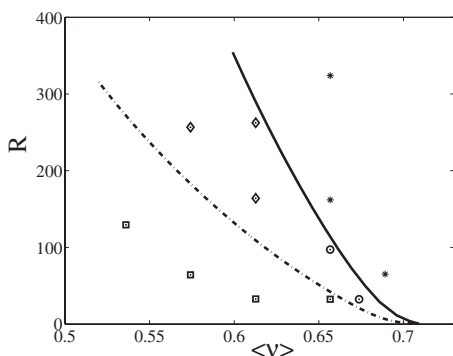


FIG. 3. $(R, \langle \nu \rangle)$ phase diagram. The uniform shear flow is stable below the dashed-dotted line, when $R < R_c(f)$ [see Eq. (4)]. The two-phase solution is possible above the solid line, when $R > R_*(f)$ [where $R_*(f)$ is computed from Eqs. (3)]. Symbols denote different solutions found in MD simulations: uniform shear flow (squares), two-phase solution (asterisks), nonuniform one-phase solutions with the density maximum in the middle of the system (rhombuses) or near the walls (circles). The number of particles in MD simulations was $N=6450 \pm 30$, and the system height was $H=(79 \pm 1)d$, while the system width L was varied in order to change the average density in the system.

ric density profile (however, other solutions were found in MD simulations [18] for moderately dense systems). Consider a solid layer located in the middle of the system, so the density maximum is at $y=0$ [as in Fig. 2(a)]. Figure 2(b) shows the density, temperature, and velocity profiles derived both from solution of Eqs. (3) (solid lines) and from MD simulations (circles). The density (the upper panel) in the central part of the system (inside the cluster) is larger than the density of viscosity divergence. This results in the $u=0$ plateau in the middle (the lower panel). An excellent agreement between the hydrodynamic theory and MD simulations can be seen.

V. PHASE DIAGRAM

Now we consider the $(R, \langle \nu \rangle)$ phase diagram, see Fig. 3. Let the average density in the system be smaller than the density of viscosity divergence n_η . If the hydrodynamic heat loss parameter R exceeds the threshold value (see the dashed-dotted line in Fig. 3)

$$R_c = \pi^2 f_1 \left(\frac{f_4(df_3/d\nu)}{(df_4/d\nu)} + \frac{f_4 f_3(df_2/d\nu)}{f_2(df_4/d\nu)} - 2f_3 \right)^{-1}, \quad (4)$$

the uniform shear flow becomes unstable (details of linear stability analysis will be given elsewhere [21]). Above this threshold, different solutions with nonuniform density and temperature profiles are realized. However, the two-phase solution is possible only when R is larger than some critical

value $R_*(f)$ [computed from Eqs. (3), the solid line in Fig. 3], so that the density contrast in the system is sufficiently large, and the maximal density is larger than n_η . An example of this solution is shown in Fig. 2 (which corresponds to the upper asterisk in Fig. 3). In order to verify the hydrodynamic predictions, we performed MD simulations in different regions of the phase diagram. We found a uniform shear flow solution (squares) below the dashed-dotted line, while above the solid line, a two-phase solution is realized (asterisks). In the intermediate region (between the two lines) there are one-phase solutions with nonuniform density (and temperature) profiles. There are two types of symmetric (with respect to a density profile) solutions, which are allowed by Eqs. (3): the density maximum can be achieved either in the middle ($y=0$), or near the walls (at $y=\pm 1/2$). MD simulations show that the system is denser in the middle when the average area fraction is not large enough (rhombuses), while for larger area fractions the density is maximum near the walls (circles).

Interestingly, the solution with solid layer in the middle of the system seems to be metastable (see also Ref. [19]). After a sufficiently long time, the cluster starts slowly moving toward one of the walls until a steady state is reached. We followed the cluster dynamics by looking at the y component of the center of mass of the system, and at the velocity in the middle $y=0$. Both quantities reach a plateau at long times, which corresponds to the position of the cluster near one of the walls. In this case, the cluster moves as a whole with a velocity which is slightly lower than the wall velocity.

VI. SUMMARY AND DISCUSSION

The dynamics of a dense rapid shear granular flow in two dimensions is analyzed both theoretically (applying granular hydrodynamics) and by means of event-driven molecular dynamics simulations. We presented a general phase diagram and described different steady-state solutions. The most interesting solution describes a flow consisting of three layers: an inner solidlike layer and two outer fluid layers. This solution is possible due to the fact that viscosity diverges at a lower density than other constitutive relations [8,11,22]. A possible direction of future research is increasing the streamwise length of the system. In this case, the layered structures may give way to wavy patterns [20]. For moderate densities, these structures can be explained theoretically [23], while for higher densities viscosity divergence should be taken into account.

ACKNOWLEDGMENTS

The author is grateful to B. Meerson and I. Aranson for fruitful discussions. The author thanks the Michigan Center for Theoretical Physics for support.

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