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Extended kinetic theory applied to dense, granular, simple shear flows

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Abstract We apply the extended kinetic theory (EKT) to the dense, simple shear flow of inelastic hard spheres. EKT is a phenomenological extension of kinetic theory which aims at incorporating in the simplest possible way the role of pre-collisional velocity correlations which are likely to occur at a concentration larger than the freezing point. The main effect of that correlation is the decrease in the rate at which fluctuating energy is dissipated in inelastic collisions. We use previously published results of numerical simulations performed using an event-driven algorithm to obtain analytical expressions for the radial distribution function at contact (which diverges at a concentration lower than the value at random close packing for sheared inelastic spheres) and the correlation length (i.e., the decreasing factor of the dissipation rate) at different values of the coefficient of restitution. With those, we show that when the diffusion of fluctuating energy of the particles is negligible, EKT implies that three branches of the analytical relation between the ratio of the shear stress to the pressure and the concentration (granular rheology) exist. Hence, for a certain value of the stress ratio, up to three corresponding values of the concentration are possible, with direct implications on the existence of multiple solutions to steady granular flows.

1 Introduction

Classic kinetic theories [14,16,23,36] have been successful in describing the behavior of granular flows at low to moderate concentration. On the other hand, at large concentration, pre-collisional velocity correlations [31,32,39] and enduring contacts among particles involved in force chains [9,37] appear; hence, both the molecular chaos and the instantaneous binary collision assumptions of classic kinetic theories fail. Unfortunately, most of the granular flows of practical interest are actually dense, and this explains why the scientific literature on the topic has grown exponentially in the recent years (e.g., see Ref. [12] for a recent review).

Substantially, two approaches have been proposed to model dense granular flows. One is entirely phenomenological and makes use of dimensional analysis to identify the dimensionless parameters governing the problem, i.e., the stress ratio, the inertial parameter, and the concentration, at least in case of rigid particles (see later in the text for more details). Physical experiments and numerical simulations are then employed to obtain a posteriori approximate algebraic relations (i.e., the granular rheology) between those parameters [9,15,26,27]. The simplicity of this approach that can be easily applied to a number of flow configurations, and even extended to deal with non-locality [28], explains its increasing popularity. The other approach is more fundamental and relies on kinetic theories by the following: (i) adding rate-independent terms borrowed

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from soil mechanics to the constitutive relations of classic kinetic theories to take into account the effects of enduring contacts [24,25,35]; (ii) extending in a phenomenological way the classic kinetic theories to take into account the decrease in the rate at which energy is dissipated in collisions due to the pre-collisional velocity correlation [19,20]; (iii) both [5].

Here, we wish to apply the extended kinetic theory (EKT) as proposed by Jenkins [19,20], and lately slightly modified and tested in a number of gravity-driven flow configurations [3,4,21,22], to the simple shear flow of inelastic, hard spheres. Many works have focused on shear flows of granular materials [1,2,6,17,40,42,45], with and without interstitial fluid. None of them though made use of EKT to solve for the flow field. It has been shown [31] that, besides the already mentioned decrease in the collisional dissipation rate, sheared inelastic granular flows show an increase in the collision frequency, which diverges at a concentration lower than the value at random close packing. The simplest possible way to incorporate this effect is to modify the radial distribution function at contact. The comparison between the analytical solution of EKT and previously published numerical simulations [39], performed using an event-driven algorithm, on frictionless hard spheres, permits to obtain the analytical form of the radial distribution function for different coefficients of restitution; and to obtain a new formulation for the correlation length (i.e., the decreasing factor in the collisional dissipation rate) that depends only on the coefficient of restitution, without requiring additional ad hoc parameters.

Besides EKT, many works have introduced a diverging length-scale to deal with correlation in granular matter. Some of them [10,33,34] focus on the spatial correlation existing in the quasi-static regime dominated by the presence of force chains, due to the rearrangements of grains after a failure, which is though different from the pre-collisional velocity correlation induced by the inelastic nature of collisions of EKT (the former is, for instance, absent in the case of frictionless hard spheres). A diverging length-scale associated with correlation that applies also to the case of frictionless hard spheres has been proposed by Lois and Carlson [34] in their force network model. Besides the fact that no analytical expression for that length-scale is proposed, the main drawback is that the diverging length-scale appears in the expression of the stress tensor (multiplying the square of the shear rate). In that case, the ratio of shear stress to the pressure would be a constant for dense granular shear flows, i.e., independent of the concentration, in contrast with the results of numerical simulations [9,31,32,38,39]. Recently [18,28], a diverging length-scale associated with particle correlation has also been introduced in a differential equation governing the spatial distribution of the inverse of the viscosity for dense granular flows. That equation has been postulated to take into account the influence of the boundaries (non-locality) in the context of the phenomenological rheology based on the inertial parameter. Once again, that correlation is different from the pre-collisional velocity correlation of EKT, given that, for instance, the former is absent in the case of simple shear flows.

2 Theory

We focus on simple shear flows of hard spheres in the absence of external forces (Fig. 1). We take x and y to be the directions parallel and perpendicular to the flow, respectively. The only component of the local mean velocity vector is u, while ν is the local value of the volume concentration. Without loss of generality, we take the particle diameter and density to be unity. The particles are characterized through the coefficient of restitution e, i.e., the ratio of the magnitude of their relative velocity after and before a collision. The momentum balances indicate that both the particle pressure p and the particle shear stress s are constant in the flow field. The balance of the fluctuating energy reduces to

$$su' - \Gamma = 0, \tag{1}$$

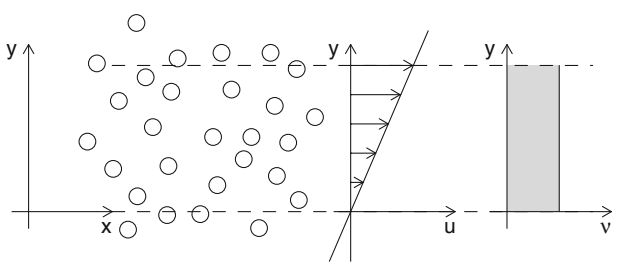

Fig. 1 Sketch of the flow configuration

Table 1 Constitutive relations from kinetic theory

$p = f_1 T$
$f_1 = 4\nu G F$
$G = \nu g_0$
$F = \frac{1+e}{2} + \frac{1}{4G}$
$s = f_2 T^{1/2} u'$
$f_2 = \frac{8J\nu G}{5\pi^{1/2}}$
$J = \frac{1+e}{2} + \frac{\pi}{32G^2} \frac{[5+2G(3e-1)(1+e)][5+4G(1+e)]}{24-6(1-e)^2-5(1-e^2)}$
$\Gamma = f_3 \frac{T^{3/2}}{L}$
$f_3 = \frac{12\nu G(1-e^2)}{\pi^{1/2}}$

where Γ is the rate of collisional dissipation. Here and in what follows, a prime indicates the derivative along y. The two terms on the left-hand side of Eq. (1) represent the energy production and dissipation, respectively.

Kinetic theories provide the closures to the problem, i.e., the constitutive relations for the pressure, the shear stress, and the rate of collisional dissipation. Here, we adopt the expressions derived by Ref. [14], summarized in Table 1, ignoring their small term c^* and using the notations of Ref. [22]. There, T is the granular temperature (one-third of the mean square of the particle velocity fluctuations), and g_0 is the radial distribution function at contact. As anticipated, EKT takes into account the fact that, when repeated collisions induce correlated motion among the particles, the rate at which energy is dissipated decreases by the factor L (correlation length), whose expression reads [20]

$$L = \max\left(L^* \frac{u'}{T^{1/2}}, 1\right), \tag{2}$$

where the coefficient L^* is a function of the concentration and the particle properties. Equation (2) ensures that, when the molecular chaos assumption holds, $L = 1$, i.e., one diameter, as in classic kinetic theories. Jenkins and Berzi [21] suggested to use

$$L^* = \frac{1}{2} c G^{1/3}, \tag{3}$$

where c is a material coefficient of order unity. The presence of this additional parameter, whose physical meaning is unclear, represents a weakness of the theory. Also the determination of the most suitable expression for the radial distribution function at contact for inelastic particles under shear is still an open issue [31,39].

Mitarai and Nakanishi [39] performed event-driven numerical simulations on shear flows of inelastic hard spheres in absence of gravity, using Lees–Edwards boundary conditions [11] along the direction perpendicular to the flow. In this case, the shear rate u', the granular temperature and the concentration are constant in the flow field (Fig. 1). Using the constitutive relation for the pressure of Table 1,

$$g_0 = \frac{1}{2\nu(1+e)} \left(\frac{p}{\nu T} - 1\right). \tag{4}$$

Hence, it is possible to obtain the radial distribution function at contact from the measured values of pressure, granular temperature, and concentration. This differs from the approach of Refs. [39] and [31], where the radial distribution function at contact was obtained in a more rigorous way from the measured collisional frequency. However, the evaluation of g_0 using Eq. (4) ensures that kinetic theory correctly predicts the particle pressure. Figure 2 shows the dependence of g_0 on the concentration obtained from Eq. (4), using the measurements of Ref. [39] at three values of the coefficient of restitution ($e = 0.7$, 0.92, and 0.98). The numerical values can be reproduced using an expression in the form suggested by Ref. [44],

$$g_0 = \frac{a}{\nu_p - \nu}, \tag{5}$$

where a is a material coefficient and ν_p represents the concentration at which the radial distribution function at contact is singular and the pressure diverges. That concentration would coincide with the concentration at

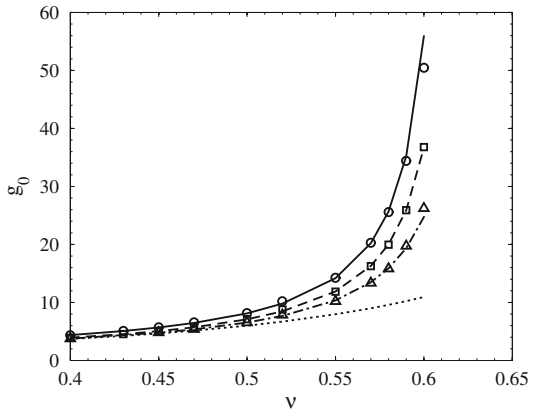

Fig. 2 Dependence of the radial distribution function at contact on the concentration obtained from pressure measurements in numerical simulations (*symbols*) and Eq. (5) (*lines*) when $e = 0.7$ (*circles* and *solid line*); $e = 0.92$ (*squares* and *dashed line*); $e = 0.98$ (*triangles* and *dot-dashed line*). The *dotted line* represents the expression of Ref. [7]

Table 2 Values of the singularity in the radial distribution function at different values of the coefficient of restitution

e	a	ν_p	ν_s
0.70	0.95	0.617	0.619
0.92	0.88	0.624	0.625
0.98	0.89	0.636	0.627

random close packing for elastic particles [43,44]. The values of a and ν_p, obtained from linear regression, for the three values of the coefficient of restitution investigated in Ref. [39] are reported in Table 2. Also shown in Fig. 2 is the widely used radial distribution function at contact of Ref. [7]. It is worth emphasizing that Eq. (5) cannot apply at low concentration, given that it is different from unity when $\nu = 0$. Also, Table 2 confirms that ν_p depends on the degree of inelasticity, unlike suggested in Ref. [8].

With Eq. (1) and the constitutive relations of Table 1, the correlation length can be written as

$$L = \max\left(\frac{f_3 T^{3/2}}{su'}, 1\right) \tag{6}$$

and can be obtained from measured values of concentration, shear stress, and granular temperature, at fixed shear rate, if Eq. (5) is used in the expression of f_3 of Table 1. For simple shear flows, the correlation length is only a function of the concentration and the material properties, given that, using Eqs. (6) and (2) and the constitutive relations of Table 1,

$$L = \max\left(\frac{f_3^{1/3}}{f_2^{1/3}} L^{*2/3}, 1\right). \tag{7}$$

Figure 3 shows the correlation length as a function of the concentration obtained using the measurements of Ref. [39] in Eq. (6). Below the concentration at the freezing point $\nu_f = 0.49$ [44], the correlation length is equal to one, indicating that the particle motion is uncorrelated (molecular chaos). Above ν_f, the correlation length increases linearly with g_0. We propose the following analytical expression for L,

$$L = \max\left[\frac{2(1-e)}{15}(g_0 - g_{0,f}) + 1, 1\right], \tag{8}$$

where $g_{0,f}$ is the value of g_0 at the freezing point. Figure 3 shows that Eq. (8) interpolates well the numerical values. From Eqs. (7) and (8), we obtain the expression of L^*,

$$L^* = \left(\frac{f_2}{f_3}\right)^{1/2} \left[\frac{2(1-e)}{15}(g_0 - g_{0,f}) + 1\right]^{3/2}, \tag{9}$$

that, unlike Eq. (3), contains only well-defined physical quantities.

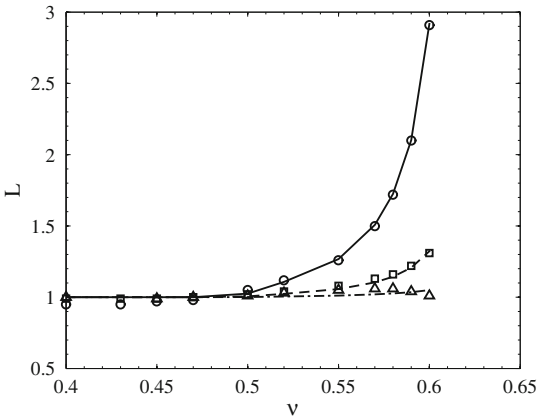

Fig. 3 Correlation length as a function of the concentration obtained from measurements in numerical simulations (*symbols*) and Eq. (8) (*lines*) when $e = 0.7$ (*circles* and *solid line*); $e = 0.92$ (*squares* and *dashed line*); $e = 0.98$ (*triangles* and *dot-dashed line*)

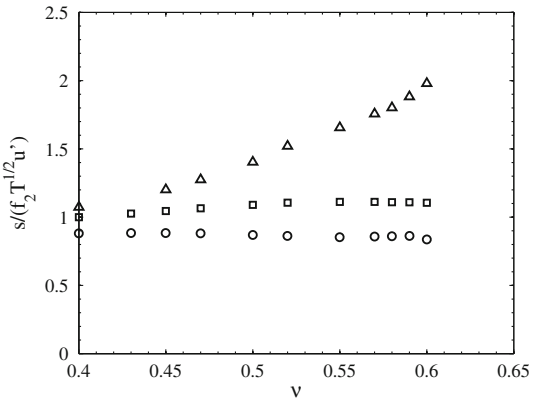

Fig. 4 Ratio of shear stress measured in numerical simulations to that obtained from the constitutive relation of kinetic theory as a function of the concentration when $e = 0.7$ (*circles*); $e = 0.92$ (*squares*); $e = 0.98$ (*triangles*)

Figure 4 depicts the ratio of the shear stress measured in the numerical simulations of [39] to that obtained from the constitutive relation of Table 1 using the measured values of concentration and granular temperature and the imposed shear rate and Eq. (5) for the radial distribution function at contact. It can be noticed, as is well known [39,41], that kinetic theories underestimate the shear stress for nearly elastic particles. On the other hand, the agreement is much more acceptable for more inelastic particles. It has been suggested that, in sheared flows, the shear viscosity diverges at a concentration lower than that at which the pressure diverges [13,29]. To check this, we have plotted in Fig. 5 the ratio $\nu^2 T^{1/2} u'/s$ as a function of the concentration obtained from the numerical simulations of Mitarai and Nakanishi [39]. In the dense limit (i.e., for $G \to \infty$), the constitutive relations of kinetic theory indicate that the ratio should be proportional to the inverse of the radial distribution function at contact, i.e., from Eq. (5), be a linear decreasing function of the volume concentration, and vanish at $\nu = \nu_p$. Indeed, Fig. 5 shows that $\nu^2 T^{1/2} u'/s$ decreases linearly with the concentration when the latter exceeds 0.5. The concentration ν_s at which $\nu^2 T^{1/2} u'/s$ vanishes (i.e., the shear viscosity diverges) for the different values of the coefficient of restitution has been obtained by linear regression and reported in Table 1. Indeed, for nearly elastic particles, the shear viscosity diverges at a concentration lower than that at which the pressure diverges, so that regions of constant velocity in the presence of a gradient of concentration and granular temperature [30] are possible. For more inelastic, and somehow more realistic, particles, instead, both the shear viscosity and the pressure diverge at the same value of concentration.

Using Eq. (6) and the constitutive relations of Table 1, we obtain the ratio of the shear stress to the pressure,

$$\frac{s}{p} = \left(\frac{f_2 f_3}{f_1^2 L} \right)^{1/2}, \tag{10}$$

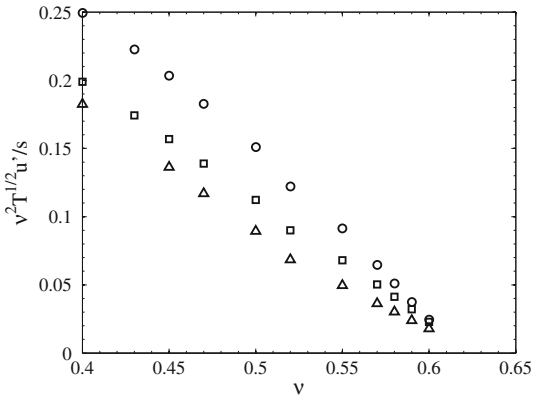

Fig. 5 Quantity $\nu^2 T^{1/2} u'/s$ obtained from numerical simulations as a function of the concentration when $e = 0.7$ (*circles*); $e = 0.92$ (*squares*); $e = 0.98$ (*triangles*)

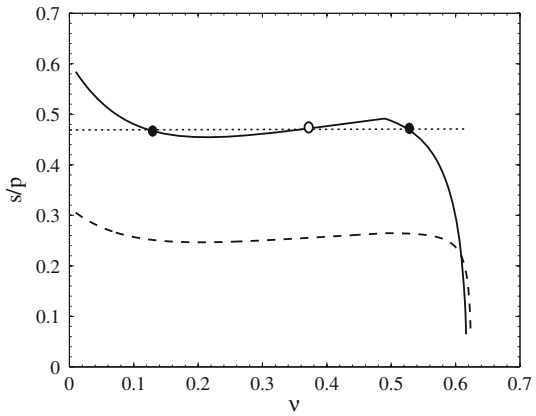

Fig. 6 Stress ratio as a function of the concentration as predicted by the extended kinetic theory for $e = 0.7$ (*solid line*) and $e = 0.92$ (*dashed line*). The *circles* indicate multiple solutions at a given level of the stress ratio

which, in the case of simple shear flows, is only a function of the concentration. Similarly, we can obtain also the relation between the so-called inertial parameter $I = u'/(p/\nu)^{1/2}$ [15] and the concentration,

$$I = \left(\frac{\nu f_3}{f_1 f_2 L} \right)^{1/2}. \tag{11}$$

Equations (10) and (11) constitute the rheology of granular materials composed of inelastic hard spheres. Although one might be tempted to use them in solving any kind of problems involving granular flows, it must be emphasized that their validity is restricted to situations for which the algebraic energy balance between production and dissipation holds. Figure 6 shows the dependence of the stress ratio on the concentration predicted by Eq. (10) at the two values of the coefficient of restitution for which the measured shear stress is well predicted by kinetic theory (Fig. 4). As expected, more inelastic particles are characterized by larger values of the stress ratio. The strong nonlinearity of Eq. (10) is reflected by the fact that up to three values of the concentration provide the same value of stress ratio. Those three values belong to three different branches of the curve: (i) the dilute branch at concentrations less than about 0.2, where the stress ratio decreases with ν; (ii) the moderate branch at concentrations in the range 0.2–0.49, where the stress ratio mildly increases with ν; (iii) the dense branch at concentrations larger than 0.49, where once again the stress ratio decreases with ν. EKT differs from classic kinetic theory in that the latter predicts that only two values of the concentration (those associated with the dilute and the moderate branches) pertain to the same value of the stress ratio.

3 Conclusion

We have applied the EKT to the simple shear flow of inelastic hard spheres. We have employed measurements of pressure, shear stress, and granular temperature at imposed concentration and shear rate from event-driven numerical simulations reported in the literature to obtain analytical expressions for the radial distribution function at contact and the correlation length in the rate of collisional dissipation at different values of the coefficient of restitution. The main results of this work are as follows: (i) the pressure diverges at a value of the concentration that decreases with the particle inelasticity, as previously reported [31]; (ii) the correlation length, employed instead of the particle diameter in the collisional rate of dissipation of EKT, is larger than one diameter at concentrations higher than the freezing point, and a simple analytical expression depending only on the coefficient of restitution is provided; (iii) the fact that the shear viscosity diverges at a concentration smaller than the pressure is a peculiar characteristic of nearly elastic particles, and not a general feature. (iv) Finally, unlike in classic kinetic theories, the analytical relation between the stress ratio and the concentration of EKT, that is possible to obtain only when the diffusion of fluctuating energy is negligible, presents three branches: one dilute for concentrations <0.2, one moderate for concentrations between 0.2 and 0.49 (freezing point), and one dense for concentrations larger than 0.49. Hence, up to three values of concentration pertain to the same value of the stress ratio. This might have important consequences, e.g., on the stability of inclined flows and the clustering phenomenon.

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