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Rheological properties in a low-density granular mixture

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Abstract

Steady simple shear flow of a low-density binary mixture of inelastic smooth hard spheres is studied in the context of the Boltzmann equation. This equation is solved by using two different and complementary approaches: a Sonine polynomial expansion and the Direct Simulation Monte Carlo method. The dependence of the shear and normal stresses as well as of the steady granular temperature on both the dissipation and the parameters of the mixture (ratios of masses, concentration, and sizes) is analyzed. In contrast to previous studies, the theory predicts and the simulation confirms that the partial temperatures of each species are different, even in the weak dissipation limit. In addition, the simulation shows that the theory reproduces fairly well the values of the shear stress and the phenomenon of normal stress differences. On the other hand, here we are mainly interested in analyzing transport in the homogeneous shear flow so that, the possible formation of particle clusters is ignored in our description.

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1. Introduction

Many features associated with dissipation in rapid granular flows can be well represented by a fluid of hard spheres with inelastic collisions. In the simplest model the grains are taken to be smooth so that the inelasticity is characterized by means

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of a constant coefficient of normal restitution. The essential difference with respect to normal fluids is the absence of energy conservation, which leads to modifications of the usual hydrodynamic equations. In recent years, the Boltzmann and Enskog equations have been generalized to account for inelastic binary collisions. These equations have been solved by means of an expansion akin to the Chapman–Enskog method up to the Navier–Stokes order and detailed expressions for the corresponding transport coefficients have been obtained [1,2]. These expressions are not restricted to the low-dissipation limit and comparison with Monte Carlo simulations indicate that the results are very accurate, even for strong dissipation [3]. In the context of multicomponent granular gases, most of the existing work appears to be based on weak dissipation approximations [4–7]. Given that the inelasticity is small, an usual assumption in these studies is to consider a single temperature variable characterizing the entire mixture. However, as one of the authors pointed out [5], the equipartition of energy is not completely justified beyond the low-dissipation limit and it is necessary to offer theories involving mixtures of granular materials in which the kinetic temperatures of species T_i are different from the mixture temperature T. As a matter of fact, recent experiments [8] and simulations [9] on *driven* granular mixtures show that the two types of grains do not attain the same granular temperature. In terms of the mean square velocities of species, this implies a violation of the classical equipartition theorem. Related findings have been reported by Garzó and Dufty [10,11] in the case of a binary mixture of inelastic hard spheres undergoing homogeneous cooling (i.e., an unforced system) and by Marconi and Puglisi [12] in the case of Maxwell molecules.

All the above works refer to near equilibrium situations. Very little is known about far from equilibrium states. This is true for both molecular and granular fluids due to the intricacy of the Boltzmann and Enskog collision operators. Nevertheless, the difficulties are even harder for granular gases since gradients in the system can be controlled by dissipation in collisions and not only by the boundary and initial conditions. Thus, for instance, a granular system with uniform boundaries at constant temperature develops spatial inhomogeneities [13]. One of the simplest far from equilibrium physical situations corresponds to the simple shear flow. Macroscopically, it is characterized by uniform density and temperature and a constant velocity profile. In the case of molecular fluids, this state is not stationary since the temperature increases monotonically in time due to viscous heating. However, for granular fluids a steady state is possible when the viscous heating is exactly balanced by the inelastic cooling. As a consequence, for a given shear rate, the temperature is a function of the restitution coefficient in the steady state. This steady state is precisely what we want to analyze here.

In the case of a one-component system, the simple shear flow has been extensively studied. Thus, Lun et al. [14] obtained the rheological properties of a dense gas for small inelasticity, while Jenkins and Richman [15] used a maximum-entropy approximation to solve the Enskog equation. An extension of the Jenkins and Richman work [15] to highly inelastic spheres has been recently made [16,17]. For low-density granular gases, Sela et al. [18] have been able to get a perturbation solution of the Boltzmann equation to third order in the shear rate, finding normal stress differences at this level of approximation. On the other hand, some progresses have been

done by using model kinetic equations in the low-density limit [19] as well as for dense gases [20]. In both works, comparison with Monte Carlo simulations shows an excellent agreement even for strong dissipation. Similar studies for multicomponent systems are more scarce. Most of them are based on a Navier–Stokes description of the hydrodynamic fields [4–7] and, therefore, they are restricted to small shear rates, which for the steady shear flow is equivalent to the low-dissipation limit. As said before, although these studies permit different temperatures for the two species, they lead to equal partial granular temperatures T_i in the quasielastic limit. A primary attempt to include temperature differences was made by Jenkins and Mancini [21], although applications of this theory which appear in the literature incorporate the assumption of equipartition of energy. Since this assumption is not valid [10,22–25] for highly inelastic spheres, a *multi-temperature* theory must be more appropriate to describe sheared granular mixtures. This fact motivates the search for theories which consistently include the possibility of temperature differences.

The aim of this paper is to get the rheological properties of a binary granular mixture subjected to the simple shear flow in the framework of the Boltzmann equation. Two complementary routes are followed. First, the set of coupled Boltzmann equations are solved by using a first-Sonine polynomial approximation with a Gaussian measure. Since the mixture is in a nonequilibrium steady state, one expects that the total energy is not equally distributed between both species. Thus, a characteristic of our solution is that the reference Gaussian distributions are defined in terms of the kinetic temperatures T_i instead of the mixture temperature T. Consequently, we do not assume a priori the equality of the three temperatures and the temperature ratio T_1/T_2 is consistently determined from the solution to the Boltzmann equations. It is found that the partial temperatures of each species are clearly different and so, energy equipartition does not hold. The consequences of this effect on the rheological properties are significant, as shown below. Once the temperature ratio is known, we get explicit expressions for the elements of the pressure tensor. The results are general and not limited in principle to weak inelasticity or specific values of the parameters of the mixture. As a second alternative and to test the reliability of the theoretical predictions, we have used the Direct Simulation Monte Carlo (DSMC) method [26] to numerically solve the Boltzmann equation in the simple shear flow. Although the DSMC method was originally devised for molecular fluids, its extension to deal with inelastic collisions is easy [27,28]. For the elements of the pressure tensor the agreement between theory and simulation turns out to be very good over a wide range of values of the restitution coefficients, mass ratios, concentration ratios and size ratios. It must be noted that in this paper we are interested in analyzing transport properties in the *uniform* shear flow. As several authors have shown [29] the simple shear flow is unstable to long enough wavelength perturbations so that clusters of particles are spontaneously developed throughout the system. Here, we will restrict ourselves to the *uniform* case, assuming that the system has reached such a state, and without paying attention to the possible formation of particle clusters (microstructure).

There is some speculation on the validity of a hydrodynamic description for granular flows beyond the weak dissipation limit and/or weakly inhomogeneous states. The concern is based on the fact that in the inelastic case the time scale for the temperature

is mainly set by the cooling rate rather than by the spatial gradients. This new time scale is much faster than the usual hydrodynamic scale so that some hydrodynamic excitations decay much slower than the granular temperature. Thus, it could happen that for finite values of the restitution coefficient there exist no time scale separation between the hydrodynamic and the fast kinetic contributions to the time evolution of the system. As a consequence, there were no "aging to hydrodynamics" or, in the kinetic theory language, "normal" solution to the Boltzmann equation. However, investigations to date [3,30] suggest that the kinetic excitations remain isolated from the hydrodynamic ones so that the later dominate on sufficiently large time scales, just as in the elastic case. This justifies the inclusion of the granular temperature as a slow or macroscopic variable. The good agreement found in this paper between our *normal* solution (obtained assuming the validity of hydrodynamics) and the simulation results supports the conclusion obtained in previous works [3,30]: a hydrodynamic description applies even at finite dissipation and strong inhomogeneity (i.e., beyond the Navier–Stokes limit).

The plan of the paper is as follows. In Section 2, the coupled Boltzmann equations and the corresponding hydrodynamic equations are recalled. The steady shear flow problem is also introduced in Section 2, while the Sonine approximation is discussed in Section 3. Section 4 deals with the Monte Carlo simulation of the Boltzmann equation particularized for steady simple shear flow. The comparison between theory and simulation is presented in Section 5 and we close the paper in Section 6 with a short discussion.

2. The Boltzmann equation and the simple shear flow

We consider a binary mixture of smooth hard spheres of masses m_1 and m_2 and diameters σ_1 and σ_2. The inelasticity of collisions are characterized by three independent constant coefficients of normal restitution α_{11}, α_{22}, and $\alpha_{12}=\alpha_{21}$, where α_{ij} is the restitution coefficient for collisions between particles of species i with j. In the low-density regime, the distribution functions $f_i(\mathbf{r},\mathbf{v};t)$ $(i=1,2)$ for the two species verify the set of nonlinear Boltzmann equations [10]

$$(\partial_t+\mathbf{v}_1\cdot\nabla)f_i(\mathbf{r},\mathbf{v}_1,t)=\sum_j J_{ij}[\mathbf{v}_1|f_i(t),f_j(t)]\,. \tag{1}$$

The Boltzmann collision operator $J_{ij}[\mathbf{v}_1|f_i,f_j]$ describing the scattering of pairs of particles is

$$J_{ij}[\mathbf{v}_1|f_i,f_j]=\sigma_{ij}^2\int d\mathbf{v}_2\int d\hat{\boldsymbol{\sigma}}\,\Theta(\hat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})(\hat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})$$
$$[\alpha_{ij}^{-2}f_i(\mathbf{r},\mathbf{v}_1',t)f_j(\mathbf{r},\mathbf{v}_2',t)-f_i(\mathbf{r},\mathbf{v}_1,t)f_j(\mathbf{r},\mathbf{v}_2,t)]\,, \tag{2}$$

where $\sigma_{ij}=(\sigma_i+\sigma_j)/2$, $\hat{\boldsymbol{\sigma}}$ is a unit vector along their line of centers, Θ is the Heaviside step function, and $\mathbf{g}_{12}=\mathbf{v}_1-\mathbf{v}_2$. The primes on the velocities denote the initial values

$\{\mathbf{v}_1', \mathbf{v}_2'\}$ that lead to $\{\mathbf{v}_1, \mathbf{v}_2\}$ following a binary collision:

$$\mathbf{v}_1' = \mathbf{v}_1 - \mu_{ji}(1+\alpha_{ij}^{-1})(\hat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})\hat{\boldsymbol{\sigma}}, \quad \mathbf{v}_2' = \mathbf{v}_2 + \mu_{ij}(1+\alpha_{ij}^{-1})(\hat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})\hat{\boldsymbol{\sigma}}\,, \tag{3}$$

where $\mu_{ij} = m_i/(m_i+m_j)$. The relevant hydrodynamic fields are the number densities n_i, the flow velocity $\mathbf{u}$, and the temperature T. They are defined in terms of moments of the distributions f_i as

$$n_i = \int d\mathbf{v}_1 f_i(\mathbf{v}_1)\,, \quad \rho\mathbf{u} = \sum_i \rho_i \mathbf{u}_i = \sum_i \int d\mathbf{v}_1\, m_i \mathbf{v}_1 f_i(\mathbf{v}_1)\,, \tag{4}$$

$$nT = \sum_i n_i T_i = \sum_i \int d\mathbf{v}_1 \frac{m_i}{3} V_1^2 f_i(\mathbf{v}_1)\,, \tag{5}$$

where $n = n_1 + n_2$ is the total number density, $\rho = \rho_1 + \rho_2 = m_1 n_1 + m_2 n_2$ is the total mass density, and $\mathbf{V}_1 = \mathbf{v}_1 - \mathbf{u}$ is the peculiar velocity. Eqs. (4) and (5) also define the flow velocity $\mathbf{u}_i$ and the partial temperature T_i of species i.

The collision operators conserve the number of particles of each species and the total momentum, but the total energy is not conserved:

$$\int d\mathbf{v}_1 J_{ij}[\mathbf{v}_1|f_i, f_j] = 0\,, \tag{6}$$

$$\sum_{i,j}\int d\mathbf{v}_1 m_i \mathbf{v}_1 J_{ij}[\mathbf{v}_1|f_i, f_j] = 0\,, \tag{7}$$

$$\sum_{i,j}\int d\mathbf{v}_1 \tfrac{1}{2} m_i V_1^2 J_{ij}[\mathbf{v}_1|f_i, f_j] = -\tfrac{3}{2} nT\zeta\,, \tag{8}$$

where ζ is identified as the "cooling rate" due to inelastic collisions among all species. At a kinetic level, it is also convenient to discuss energy transfer in terms of the "cooling rates" ζ_i for the partial temperatures T_i. They are defined as

$$\zeta_i = -\frac{2}{3n_i T_i}\sum_j \int d\mathbf{v}_1 \tfrac{1}{2} m_i V_1^2 J_{ij}[\mathbf{v}_1|f_i, f_j]\,. \tag{9}$$

The total cooling rate ζ can be written as

$$\zeta = T^{-1}\sum_i x_i T_i \zeta_i\,, \tag{10}$$

where $x_i = n_i/n$ being the molar fraction of species i.

From Eqs. (4)–(8), the macroscopic balance equations for the mixture can be obtained. They are given by

$$D_t n_i + n_i \nabla\cdot\mathbf{u} + \frac{\nabla\cdot\mathbf{j}_i}{m_i} = 0\,, \tag{11}$$

$$D_t \mathbf{u} + \rho^{-1}\nabla\cdot\mathsf{P} = 0\,, \tag{12}$$

$$D_t T - \frac{T}{n}\sum_i \frac{\nabla\cdot\mathbf{j}_i}{m_i} + \frac{2}{3n}(\nabla\cdot\mathbf{q} + \mathsf{P}:\nabla\mathbf{u}) = -\zeta T\,. \tag{13}$$

In the above equations, $D_t = \partial_t + \mathbf{u}\cdot\nabla$ is the material derivative,

$$\mathbf{j}_i = m_i \int d\mathbf{v}_1\, \mathbf{V}_1 f_i(\mathbf{V}_1) \tag{14}$$

is the mass flux for species i relative to the local flow,

$$\mathsf{P} = \sum_i \mathsf{P}_i = \sum_i \int d\mathbf{v}_1\, m_i \mathbf{V}_1\mathbf{V}_1 f_i(\mathbf{V}_1) \tag{15}$$

is the total pressure tensor, and

$$\mathbf{q} = \sum_i \mathbf{q}_i = \sum_i \int d\mathbf{v}_1\, \tfrac{1}{2} m_i V_1^2 \mathbf{V}_1 f_i(\mathbf{V}_1) \tag{16}$$

is the total heat flux. The partial contributions to the pressure tensor, P_i, and the heat flux, $\mathbf{q}_i$, coming from species i can be identified from Eqs. (15) and (16).

As said in the Introduction, here we are interested in evaluating the rheological properties of a granular binary mixture subjected to the simple shear flow. From a macroscopic point of view, this state is characterized by a constant linear velocity profile $\mathbf{u} = \mathbf{u}_i = \mathsf{a}\cdot\mathbf{r}$, where the elements of the tensor a are $a_{k\ell} = a\delta_{kx}\delta_{\ell y}$, a being the constant shear rate. In addition, the partial densities n_i and the granular temperature T are uniform, while the mass and heat fluxes vanish by symmetry reasons. Thus, the (uniform) pressure tensor is the only nonzero flux in the problem. On the other hand, the temporal variation of the granular temperature arises from the balance of two opposite effects: viscous heating and dissipation in collisions. In the steady state both mechanisms cancel each other and the temperature remains constant. In that case, according to the balance energy equation (13), the shear stress P_{xy} and the cooling rate ζ are related by

$$aP_{xy} = -\frac{3}{2}\,\zeta p\,, \tag{17}$$

where $p = nT$ is the pressure. Our aim is to analyze this steady state by means of an (approximate) analytical method as well as by performing Monte Carlo simulations of the Boltzmann equation.

The simple shear flow becomes spatially uniform when one refers the velocities of the particles to a frame moving with the flow velocity $\mathbf{u}$: $f_i(\mathbf{r},\mathbf{v}_1) \to f_i(\mathbf{V}_1)$. Consequently, the corresponding Boltzmann equations (1) read

$$-aV_{1,y}\frac{\partial}{\partial V_{1,x}} f_1(\mathbf{V}_1) = J_{11}[\mathbf{V}_1|f_1,f_1] + J_{12}[\mathbf{V}_1|f_1,f_2]\,, \tag{18}$$

$$-aV_{1,y}\frac{\partial}{\partial V_{1,x}} f_2(\mathbf{V}_1) = J_{22}[\mathbf{V}_1|f_2,f_2] + J_{21}[\mathbf{V}_1|f_2,f_1]\,. \tag{19}$$

The elements of the partial pressure tensors P_i $(i=1,2)$ can be obtained by multiplying the Boltzmann equations by $m_i V_{1,k} V_{1,\ell}$ and integrating over $\mathbf{V}_1$. The result is

$$a_{km}P_{1,\ell m} + a_{\ell m}P_{1,km} = A_{k\ell}^{11} + A_{k\ell}^{12} \quad (1\leftrightarrow 2)\,, \tag{20}$$

where

$$A_{k\ell}^{ij} = m_i \int d\mathbf{V}_1 V_{1,k} V_{1,\ell} J_{ij}[\mathbf{V}_1|f_i,f_j]\,. \tag{21}$$

From Eq. (20), in particular, one obtains

$$aP_{1,xy} = -\tfrac{3}{2}\, p_1 \zeta_1 \,, \tag{22}$$

$$aP_{1,yy} = A_{xy}^{11} + A_{xy}^{12} \,, \tag{23}$$

$$0 = A_{yy}^{11} + A_{yy}^{12} = A_{zz}^{11} + A_{zz}^{12} \,. \tag{24}$$

Here, $p_1 = n_1 T_1 = (P_{1,xx} + P_{1,yy} + P_{1,zz})/3$ is the partial pressure of species 1 and upon writing Eq. (22) we have considered the relation (8). The corresponding equations for P_2 can easily be written just by interchanging the indices 1 and 2. Thus, the determination of the elements of the partial pressure tensors P_i is a closed problem once the cooling rates ζ_i and the collisional moments $A_{k\ell}^{ij}$ are known. This requires the explicit knowledge of the velocity distribution functions f_i.

3. Approximate solution

Unfortunately, solving the Boltzmann Eqs. (18) and (19) is a formidable task and it does not seem possible to get the exact forms of the distributions f_i, even in the one-component case. A possible way to overcome such a problem is to expand f_i in a complete set of polynomials with a Gaussian measure and then truncate the series. In practice, Sonine polynomials are used. This approach is similar to the usual moment method for solving kinetic equations in the elastic case. In the context of granular gases, this strategy has been widely applied in the past few years in the one-component case as well as for multicomponent systems and excellent approximations have been obtained by retaining only the first two terms. Therefore, one can expect to get a reasonable estimate for ζ_i and $A_{k\ell}^{ij}$ by using the following approximation for f_i:

$$f_i(\mathbf{V}_1) \to f_{i,M}(\mathbf{V}_1) \left[1 + \frac{m_i}{2T_i} C_{i,k\ell} \left(V_{1,k} V_{1,\ell} - \frac{1}{3} V_1^2 \delta_{k\ell} \right)\right] \,, \tag{25}$$

where $f_{i,M}$ is a Maxwellian distribution at the temperature of the species i, i.e.,

$$f_{i,M}(\mathbf{V}_1) = n_i \left(\frac{m_i}{2\pi T_i}\right)^{3/2} \exp\left(-\frac{m_i V^2}{2T_i}\right) \,. \tag{26}$$

As we will show later, in general the three temperatures T, T_1, and T_2 are different in the inelastic case. For this reason we choose the parameters in the Maxwellians so that it is normalized to n_i and provides the exact second moment of f_i. The Maxwellians $f_{i,M}$ for the two species can be quite different due to the temperature differences. This aspect is essential in our two-temperature theory and has not been taken into account in all previous studies. The coefficient C_i can be identified by requiring the moments with respect to $V_{1,k} V_{1,\ell}$ of the trial function (25) to be the same as those for the exact distribution f_i. This leads to

$$C_{i,k\ell} = \frac{P_{i,k\ell}}{p_i} - \delta_{k\ell} \,. \tag{27}$$

With this approximation, the integrals appearing in the expressions of ζ_i and $A_{k\ell}^{ij}$ can be evaluated and the details are given in Appendices A and B.

In order to express the solution of the system of equations for the pressure tensor, it is convenient to introduce dimensionless quantities. To do that, we have to take a time unit. In general there are several characteristic times in a binary mixture, so that the choice of the adequate time depends on the case of interest (tracer limit, disparate-mass mixture, etc.). Since here our description applies for arbitrary mass, concentration, and size ratios, we take, for simplicity, an effective collision frequency ν given by $\nu=\sqrt{\pi}n\sigma_{12}^2 v_0$, where $v_0=\sqrt{2T(m_1+m_2)/m_1m_2}$ is a thermal velocity defined in terms of the global temperature T. Therefore, we introduce the reduced cooling rates $\zeta_i^*=\zeta_i/\nu$, the reduced temperature $T^*=v^2/a^2$, and the reduced pressure tensors $\mathsf{P}_i^*=\mathsf{P}_i/x_i p$. The (reduced) total pressure tensor is $\mathsf{P}^*=\mathsf{P}/p=x_1\mathsf{P}_1^*+x_2\mathsf{P}_2^*$. Notice that, for given values of the parameters of the mixture, T^* and P^* are functions of the restitution coefficients α_{ij} only.

According to the symmetry of the problem, $P_{i,xz}=P_{i,yz}=0$, so that the nonzero elements are $P_{i,xx}$, $P_{i,yy}$, $P_{i,zz}$, and $P_{i,xy}=P_{i,yx}$. The three normal elements are not independent since $P_{i,xx}^*+P_{i,yy}^*+P_{i,zz}^*=3\gamma_i$, where the temperature ratios $\gamma_i=T_i/T$ are given by

$$\gamma_1=\frac{\gamma}{1+x_1(\gamma-1)},\quad \gamma_2=\frac{1}{1+x_1(\gamma-1)}\,, \tag{28}$$

with $\gamma=T_1/T_2=\gamma_1/\gamma_2$. Eqs. (28) can be easily obtained from the first equality of Eq. (5). The temperature ratio γ provides information about how the kinetic energy is distributed between both species. The fact that in general $T_1\neq T_2$ does not mean that there are additional hydrodynamic degrees of freedom since the partial kinetic temperatures T_i can be written in terms of the average temperature T, but the temperature ratio is a function of dissipation and leads to new effects (not previously considered) on the rheological properties, as shown below. In addition, according to Eq. (24), $P_{i,yy}^*=P_{i,zz}^*$. Consequently, the partial pressure tensors have four relevant elements, say for instance: $\mathscr{P}\equiv\{P_{1,yy}^*,P_{2,yy}^*,P_{1,xy}^*,P_{2,xy}^*\}$. Taking into account the results derived in the Appendices, Eqs. (23) and (24) (plus their corresponding counterparts for species 2) can be written as

$$\mathscr{L}\mathscr{P}=\mathscr{Q}\,, \tag{29}$$

where $\mathscr{L}$ is the 4×4 matrix

$$\mathscr{L}=\begin{pmatrix} 1 & 0 & -(G_{11}+G_{12})\nu/a & -H_{12}\nu/a \\ 0 & 1 & -H_{21}\nu/a & -(G_{22}+G_{21})\nu/a \\ -(G_{11}+G_{12}) & -H_{12} & 0 & 0 \\ -H_{21} & -(G_{22}+G_{21}) & 0 & 0 \end{pmatrix}, \tag{30}$$

and

$$\mathscr{Q}=\begin{pmatrix} 0 \\ 0 \\ F_{11}+F_{12} \\ F_{22}+F_{21} \end{pmatrix}. \tag{31}$$

Here, the functions F_{ij}, G_{ij}, and H_{ij} are defined in the Appendix B. The solution to Eq. (29) is

$$\mathscr{P} = \mathscr{L}^{-1}\mathscr{Q}\,. \tag{32}$$

Eq. (32) gives the nonzero elements of the pressure tensors P_i^* in terms of the reduced temperature T^* (or the reduced shear rate a/v), the temperature ratio γ, the restitution coefficients and the parameters of the mixture. The dependence of T^* on the coefficients α_{ij} can be obtained from the energy balance equation (17)

$$T^{*-1/2} = -\frac{3}{2}\frac{\zeta^*}{P_{xy}^*} = -\frac{3}{2}\frac{x_1\gamma_1\zeta_1^* + x_2\gamma_2\zeta_2^*}{x_1 P_{1,xy}^* + x_2 P_{2,xy}^*}\,. \tag{33}$$

Finally, when Eqs. (32) and (33) are used in Eq. (22) (or its counterpart for the species 2), one gets a *closed* equation for the temperature ratio γ, that can be solved numerically. In reduced units, this equation can be written as

$$\gamma = \frac{\zeta_2^*}{\zeta_1^*}\frac{P_{1,xy}^*}{P_{2,xy}^*}\,. \tag{34}$$

In the elastic limit ($\alpha_{ij}=1$), we recover previous results derived for molecular gases [31]. A simple and interesting case corresponds to the case of mechanically equivalent particles ($m_1=m_2$, $\alpha_{11}=\alpha_{22}=\alpha_{12}\equiv\alpha$, $\sigma_{11}=\sigma_{22}$). In this limit, Eqs. (32)–(34) leads to $\gamma=1$, $\mathsf{P}^*=\mathsf{P}_1^*=\mathsf{P}_2^*$, with

$$P_{yy}^* = \frac{2}{3}\frac{2+\alpha}{3-\alpha}\,, \tag{35}$$

$$P_{xy}^* = -\frac{5}{3}\frac{2+\alpha}{(1+\alpha)(3-\alpha)^2}\frac{a}{v}\,, \tag{36}$$

$$P_{xx}^* = 3 - 2P_{yy}^*\,, \tag{37}$$

and

$$T^{*-1} \equiv \frac{a^2}{v^2} = \frac{3}{5}\frac{(1+\alpha)(3-\alpha)^2}{2+\alpha}(1-\alpha^2)\,. \tag{38}$$

These expressions differ from the results derived in Ref. [19] by using a model kinetic equation. However, for practical purposes, the discrepancies between both approximations are quite small, even for moderate values of the restitution coefficient. It is also interesting to consider the limit of weak dissipation ($1-\alpha_{ij}\ll 1$), in which case it is possible to get analytical results. For the sake of simplicity, let us assume that all the particles have the same coefficient of restitution, namely, $\alpha_{11}=\alpha_{22}=\alpha_{12}\equiv\alpha$. To get the first-order corrections in the quasielastic limit, we introduce the perturbation parameter $\varepsilon\equiv(1-\alpha^2)^{1/2}$ and perform a series expansion around $\varepsilon=0$. The leading term of the reduced shear rate a/v (which is a measure of the steady granular temperature) is of the form

$$\frac{a}{v} = a_0(1-\alpha^2)^{1/2} + \cdots\,. \tag{39}$$

Next, the temperature ratio and the relevant elements of the (partial) pressure tensors can be written in the form

$$\gamma = 1 + \gamma_0(1-\alpha^2) + \cdots , \tag{40}$$

$$P^*_{i,yy} = 1 + P^{(2)}_{i,yy}(1-\alpha^2) + \cdots , \tag{41}$$

$$P^*_{i,xx} = 1 + P^{(2)}_{i,xx}(1-\alpha^2) + \cdots , \tag{42}$$

$$P^*_{i,xy} = P^{(1)}_{i,xy}(1-\alpha^2)^{1/2} + \cdots . \tag{43}$$

In these equations, a_0, γ_0, and $P^{(r)}_{i,k\ell}$ are dimensionless coefficients that depend on the ratios of mass, concentrations and sizes. For symmetry reasons, the expansion of $P^*_{i,xy}$ has only odd powers, while those of the normal stresses (and of the temperature ratio) have only even powers. The explicit expressions of a_0, γ_0, and $P^{(r)}_{i,k\ell}$ can be easily obtained by considering only terms through second order in ε in the general solution (32) and in Eqs. (33) and (34). The final expressions of these quantities will be omitted here since they are very large and not very illuminating.

In summary, by using the Sonine approximation (25), we have explicitly determined the rheological properties of the mixture as well as the reduced shear rate and the temperature ratio as functions of dissipation and mechanical parameters of the mixture. These theoretical predictions will be compared with those obtained from Monte Carlo simulations in Section 5.

4. Monte Carlo simulation

From a numerical point of view, the DSMC method [26] is the most convenient algorithm to study nonequilibrium phenomena in the low-density regime. It was devised to mimic the dynamics involved in the Boltzmann collision term. The extension of the DSMC method to deal with inelastic collisions is straightforward [20,27,28], and here we have used it to numerically solve the Boltzmann equation in the simple shear flow. In addition, since the simple shear flow is spatially homogeneous in the local Lagrangian frame, the simulation method becomes especially easy to implement. This is an important advantage with respect to molecular dynamics simulations. On the other hand, the restriction to this homogeneous state prevents us from analyzing the possible instability of simple shear flow or the formation of clusters or microstructures.

The DSMC method as applied to the simple shear flow is as follows. The velocity distribution function of the species i is represented by the peculiar velocities $\{\mathbf{V}_k\}$ of N_i "simulated" particles:

$$f_i(\mathbf{V},t) \to n_i \frac{1}{N_i}\sum_{k=1}^{N_i} \delta(\mathbf{V}-\mathbf{V}_k(t)) . \tag{44}$$

Note that the number of particles N_i must be taken according to the relation $N_1/N_2 = n_1/n_2$. At the initial state, one assigns velocities to the particles drawn from the Maxwell–Boltzmann probability distribution:

$$f_i(\mathbf{V},0) = n_i \pi^{-3/2} V_{0i}^{-3}(0) \exp\left(-V^2/V_{0i}^2(0)\right), \tag{45}$$

where $V_{0i}^2(0) = 2T(0)/m_i$ and $T(0)$ is the initial temperature. To enforce a vanishing initial total momentum, the velocity of every particle is subsequently subtracted by the amount $N_i^{-1}\sum_k \mathbf{V}_k(0)$. In the DSMC method, the free motion and the collisions are uncoupled over a time step Δt which is small compared with the mean free time and the inverse shear rate. In the local Lagrangian frame, particles of each species ($i=1,2$) are subjected to the action of a non-conservative inertial force $\mathbf{F}_i = -m_i\, \mathsf{a}\cdot\mathbf{V}$. This force is represented by the terms on the left-hand side of Eqs. (18) and (19). Thus, the free motion stage consists of making $\mathbf{V}_k \to \mathbf{V}_k - \mathsf{a}\cdot\mathbf{V}_k\Delta t$. In the collision stage, binary interactions between particles of species i and j must be considered. To simulate the collisions between particles of species i with j a sample of $\frac{1}{2}N_i\omega_{\max}^{(ij)}\Delta t$ pairs is chosen at random with equiprobability. Here, $\omega_{\max}^{(ij)}$ is an upper bound estimate of the probability that a particle of the species i collides with a particle of the species j. Let us consider a pair $\{k,\ell\}$ belonging to this sample. Here, k denotes a particle of species i and ℓ a particle of species j. For each pair $\{k,\ell\}$ with velocities $\{\mathbf{V}_k,\mathbf{V}_\ell\}$, the following steps are taken: (1) a given direction $\hat{\boldsymbol{\sigma}}_{k\ell}$ is chosen at random with equiprobability; (2) the collision between particles k and ℓ is accepted with a probability equal to $\Theta(\mathbf{g}_{k\ell}\cdot\hat{\boldsymbol{\sigma}}_{k\ell})\omega_{k\ell}^{(ij)}/\omega_{\max}^{(ij)}$, where $\omega_{k\ell}^{(ij)} = 4\pi\sigma_{ij}^2 n_j|\mathbf{g}_{k\ell}\cdot\hat{\boldsymbol{\sigma}}_{k\ell}|$ and $\mathbf{g}_{k\ell} = \mathbf{V}_k - \mathbf{V}_\ell$; (3) if the collision is accepted, postcollisional velocities are assigned to both particles according to the scattering rules:

$$\mathbf{V}_k \to \mathbf{V}_k - \mu_{ji}(1+\alpha_{ij})(\mathbf{g}_{k\ell}\cdot\hat{\boldsymbol{\sigma}}_{k\ell})\hat{\boldsymbol{\sigma}}_{k\ell}\,, \tag{46}$$

$$\mathbf{V}_\ell \to \mathbf{V}_\ell + \mu_{ij}(1+\alpha_{ij})(\mathbf{g}_{k\ell}\cdot\hat{\boldsymbol{\sigma}}_{k\ell})\hat{\boldsymbol{\sigma}}_{k\ell}\,. \tag{47}$$

In the case that in one of the collisions $\omega_{k\ell}^{(ij)} > \omega_{\max}^{(ij)}$, the estimate of $\omega_{\max}^{(ij)}$ is updated as $\omega_{\max}^{(ij)} = \omega_{k\ell}^{(ij)}$. The procedure described above is performed for $i=1,2$ and $j=1,2$.

In the course of the simulations, one evaluates the total pressure tensor and the partial temperatures. They are given as

$$\mathsf{P} = \sum_{i=1}^{2}\frac{m_i n_i}{N_i}\sum_{k=1}^{N_i}\mathbf{V}_k\mathbf{V}_k\,, \tag{48}$$

$$T_i = \frac{m_i}{3N_i}\sum_{k=1}^{N_i}\mathbf{V}_k^2\,. \tag{49}$$

To improve the statistics, the results are averaged over a number $\mathcal{N}$ of independent realizations or replicas. In our simulations we have typically taken a total number of particles $N = N_1 + N_2 = 10^5$, a number of replicas $\mathcal{N} = 10$, and a time step $\Delta t = 3\times 10^{-3}\lambda_{11}/V_{01}(0)$, where $\lambda_{11} = (\sqrt{2}\pi n_1\sigma_{11}^2)^{-1}$ is the mean free path for collisions 1–1.

A complete presentation of the results is complex since there are many parameters involved: $\{\alpha_{ij}, m_1/m_2, n_1/n_2, \sigma_{11}/\sigma_{22}\}$. For the sake of concreteness, henceforth

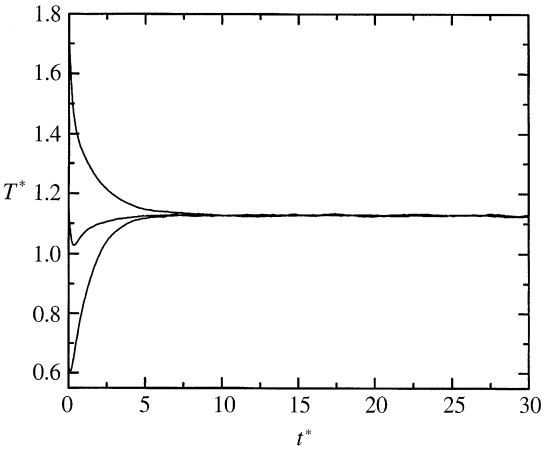

Fig. 1. Time evolution of the reduced granular temperature $T^*(t) = v^2(t)/a^2$ as obtained from Monte Carlo simulation of the Boltzmann equation for $\alpha = 0.75$, $\sigma_{11} = \sigma_{22}$, $n_1/n_2 = 1/3$, $m_1/m_2 = 4$, and starting from three different initial conditions. Time is measured in units of $\lambda_{11}/V_{01}(0)$.

we will consider the case $\alpha_{11} = \alpha_{22} = \alpha_{12} \equiv \alpha$. In the steady state, the reduced quantities T^*, γ_i, and P^* are independent of the initial state for given values of the restitution coefficient and the ratios of mass, concentration and sizes. To illustrate it, in Fig. 1 we present the time evolution of $T^*(t)$ for $\alpha = 0.75$, $\sigma_{11}/\sigma_{22} = 1$, $m_1/m_2 = 4$, $n_1/n_2 = 1/3$ and three different initial conditions. Time is measured in units of $\lambda_{11}/V_{01}(0)$. After an initial transient period, all curves converge to the same steady value, as predicted by the solution described in Section 3. The same qualitative behavior has been found for the temperature ratio and the elements of the reduced pressure tensor. Therefore, in the following we will focus on the dependence of the steady values of the reduced quantities on the restitution coefficient α and the parameters of the mixture, once we have checked that they do not depend on the initial state.

5. Comparison between theory and Monte Carlo simulations

In this section we compare the predictions of the Sonine approximation with the results obtained from the DSMC method. Our goal is to explore the dependence of a^*, $\gamma = T_1/T_2$ and the nonzero elements of P^* on α, the mass ratio $\mu \equiv m_1/m_2$, the concentration ratio $\delta \equiv n_1/n_2$, and the ratio of sizes $w \equiv \sigma_{11}/\sigma_{22}$.

First, we will investigate the dependence of the relevant quantities on α and μ for given values of δ and w. Recent molecular dynamics simulations for a dilute monocomponent system of smooth inelastic hard disks [32] have supported an "equation of state" to a sheared granular system in which the steady (reduced) temperature T^* can be closely fitted by a linear function of $(1-\alpha^2)^{-1}$. Similar results have been obtained from kinetic models of the Boltzmann [19] and Enskog [20] equations. An

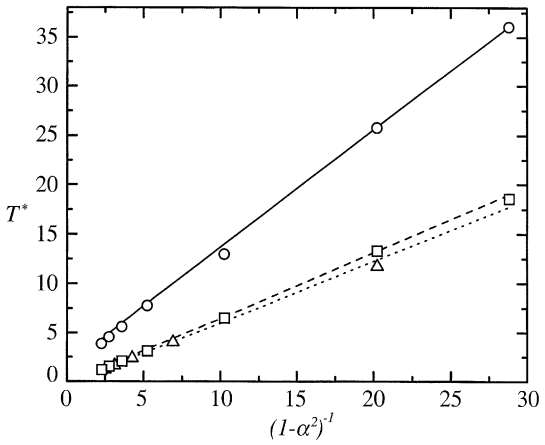

Fig. 2. Plot of the reduced granular temperature $T^* = v^2/a^2$ versus the parameter $(1-\alpha^2)^{-1}$ as obtained from simulation (symbols) and the Sonine approximation (lines), for $w = \sigma_{11}/\sigma_{22} = 1$, $\delta = n_1/n_2 = 1$ and three different values of the mass ratio $\mu = m_1/m_2$: $\mu = 10$ (— and ◯); $\mu = 2$ (- - - and □), and $\mu = 1$ (··· and △).

interesting question is whether this simple relationship can be extended to the case of multicomponent systems. The results obtained here (both from the simulations and from the kinetic theory analysis) for mixtures of different masses, concentrations or sizes show that T^* is indeed a *quasi* linear function of $(1-\alpha^2)^{-1}$. As an illustrative example, we consider the case $w = 1$, $\delta = 1$ (equimolar mixture), and three different values of the mass ratio $\mu = 1$, 2, and 10. Fig. 2 shows T^* versus $(1-\alpha^2)^{-1}$ as obtained from the simulations (symbols) and from the Sonine approximation (lines). It is evident that the kinetic theory has an excellent agreement with the simulation results and also that T^* is practically linear in $(1-\alpha^2)^{-1}$ whatever the mass ratio considered is. The slope of the straight lines increases as the disparity of masses increases.

The temperature ratio and the nonzero elements of the pressure tensor are plotted in Figs. 3 and 4 (a–d), respectively, as a function of the dissipation parameter α for the same cases as those considered in Fig. 2. The curves corresponding to $\mu < 1$ can be easily inferred from them. Given the intrinsic connection between the velocity gradient and dissipation in the simple shear flow problem, energy nonequipartition is expected as the restitution coefficient decreases (which means here nonequilibrium steady states). Fig. 3 clearly shows that, except for mechanically equivalent particles, the partial temperatures are different, even for moderate dissipation (say $\alpha \simeq 0.9$). The effect of temperature differences is generic of multicomponent dissipative systems and is consistent with results recently derived in the homogeneous cooling state [10,25] as well as in driven systems [8,9]. The extent of the equipartition violation depends on the concentrations and the mechanical differences of the particles (e.g., masses, sizes, restitution coefficients), and is greater when the differences are large. The agreement between theory and simulation is again excellent. With respect to the pressure tensor,

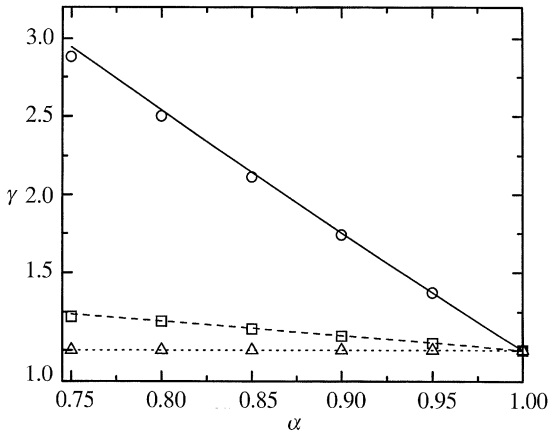

Fig. 3. Plot of the temperature ratio $\gamma = T_1/T_2$ as a function of the restitution coefficient α as obtained from simulation (symbols) and the Sonine approximation (lines). We have considered $w=\sigma_{11}/\sigma_{22}=1$, $\delta=n_1/n_2=1$ and three different values of the mass ratio $\mu=m_1/m_2$: $\mu=10$ (— and ◯); $\mu=2$ (- - - and □), and $\mu=1$ (··· and △).

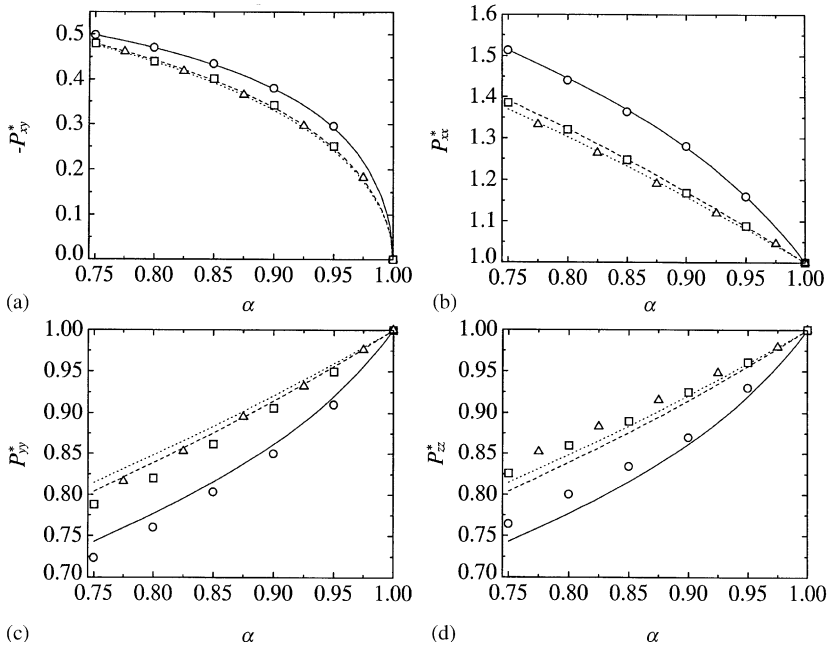

Fig. 4. Plot of the reduced elements of the pressure tensor: (a) $-P^*_{xy} = -P_{xy}/p$; (b) $P^*_{xx} = P_{xx}/p$; (c) $P^*_{yy} = P_{yy}/p$ and (d) $P^*_{zz} = P_{zz}/p$ versus the restitution coefficient α as obtained from simulation (symbols) and the Sonine approximation (lines). We have considered $w=\sigma_{11}/\sigma_{22}=1$, $\delta=n_1/n_2=1$ and three different values of the mass ratio $\mu=m_1/m_2$: $\mu=10$ (— and ◯); $\mu=2$ (- - - and □), and $\mu=1$ (··· and △).

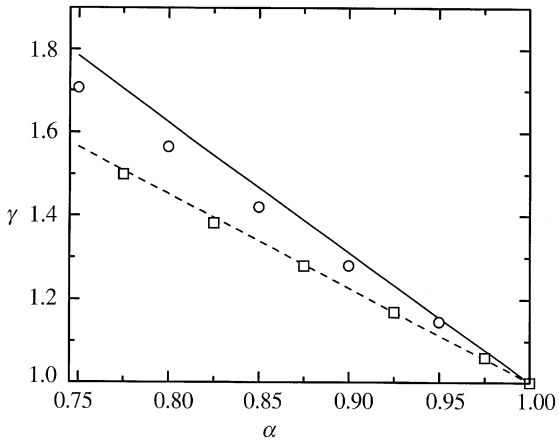

Fig. 5. Plot of the temperature ratio $\gamma = T_1/T_2$ as a function of the restitution coefficient α as obtained from simulation (symbols) and the Sonine approximation (lines). We have considered $w = \sigma_{11}/\sigma_{22} = 1$, $\mu = m_1/m_2 = 4$ and two different values of the concentration ratio $\delta = n_1/n_2$: $\delta = 1/3$ (— and ◯), and $\delta = 3$ (- - - and □).

Fig. 4 (a–d), we see that the theory captures well the main trends observed for the rheological properties. At a quantitative level, the agreement is better in the case of the shear stress P^*_{xy} and the normal element P^*_{xx}, while the discrepancies for the normal stresses P^*_{yy} and P^*_{zz} are larger than in the case of the temperature ratio, especially as the restitution coefficient decreases. On the other hand, the theory only predicts normal stress differences in the plane of shear flow ($P^*_{xx} \neq P^*_{yy} = P^*_{zz}$) while the simulation also shows that there is anisotropy in the plane perpendicular to the flow velocity, $P^*_{zz} > P^*_{yy}$. This kind of anisotropy has also been observed in molecular dynamics simulations of shear flows [33]. Nevertheless, these relative normal stress differences in this plane are very small and decrease as α increases.

The influence of the concentration ratio δ on the temperature ratio and the rheological properties is shown in Figs. 5 and 6 (a–d), respectively, for $w = 1$, $\mu = 4$, and two values of δ: $\delta = 1/3$ and $\delta = 3$. We observe again a strong dependence of the temperature ratio γ on dissipation. For a given value of α, the temperature ratio increases as the molar fraction of the heavy species decreases. Concerning shear stresses, we see that they are practically independent of the concentration ratio since all the curves collapse in a common curve. A more significant influence is observed for the normal stresses. In general, the agreement with the theory is good although the discrepancies are more important in the case of $\delta = 1/3$. Finally, the influence of the size of the particles on the rheological properties is illustrated in Fig. 7 (a–d). We consider an equimolar mixture ($\delta = 1$) of particles of equal mass ($\mu = 1$) for two different values of the size ratio: $w = 1$, and $w = 2$. We see that similar conclusions to those previously found in Figs. 3–6 are obtained when one considers mixtures of particles of different sizes.

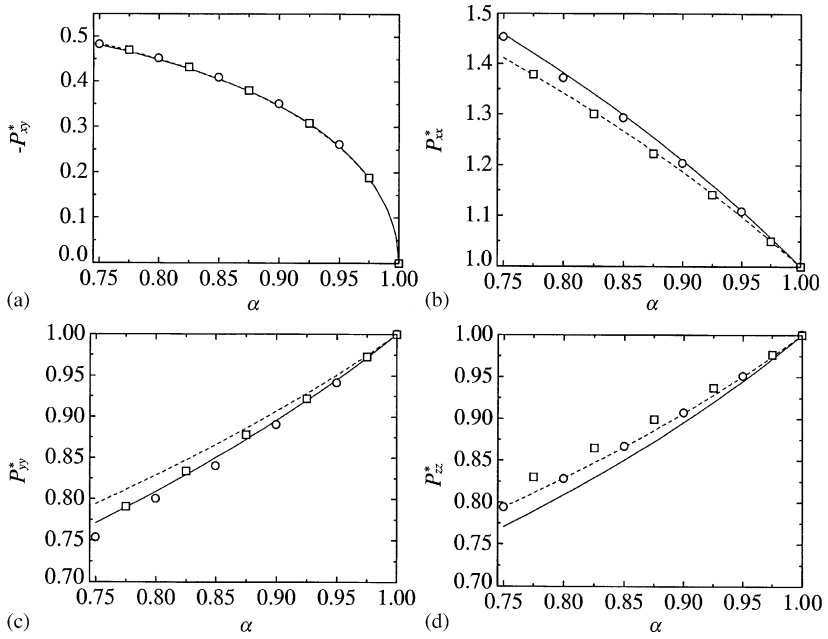

Fig. 6. Plot of the reduced elements of the pressure tensor: (a) $-P^*_{xy} = -P_{xy}/p$; (b) $P^*_{xx} = P_{xx}/p$; (c) $P^*_{yy}=P_{yy}/p$ and (d) $P^*_{zz}=P_{zz}/p$ versus the restitution coefficient α as obtained from simulation (symbols) and the Sonine approximation (lines). We have considered $w=\sigma_{11}/\sigma_{22}=1$, $\mu=m_1/m_2=4$ and two different values of the concentration ratio $\delta=n_1/n_2$: $\delta=1/3$ ((—) and ◯), and $\delta=3$ (- - - and □).

6. Discussion

In this paper, we have addressed the problem of a low-density granular mixture constituted by smooth inelastic hard spheres and subjected to a linear shear flow $u_x=ay$. We are interested in the steady state where the effect of viscosity is compensated for by the dissipation in collisions. Our description applies for arbitrary values of the shear rate a or the inelasticity of the system and no restriction on the values of masses, concentrations and sizes are imposed in the system. The study has been made by using two different and complementary routes. On the one hand, the set of coupled Boltzmann equations are solved by means of a Sonine polynomial approximation and, on the other hand, Monte Carlo simulations are performed to numerically solve the Boltzmann equations. Given that the partial temperatures T_i of each species can be different, the reference Maxwellians in the Sonine expansion are defined at the temperature for that species. This is one of the new features of our expansion. On the other hand, to put this work in a proper context, it must be noticed that we have restricted our considerations to states in which the only gradient is the one associated with the shear rate so that density and velocity fluctuations are not allowed in the numerical simulation.

We have focused on the analysis of the dependence of the steady (reduced) temperature T^* and the (reduced) pressure tensor P^* on the coefficients of restitution α_{ij}

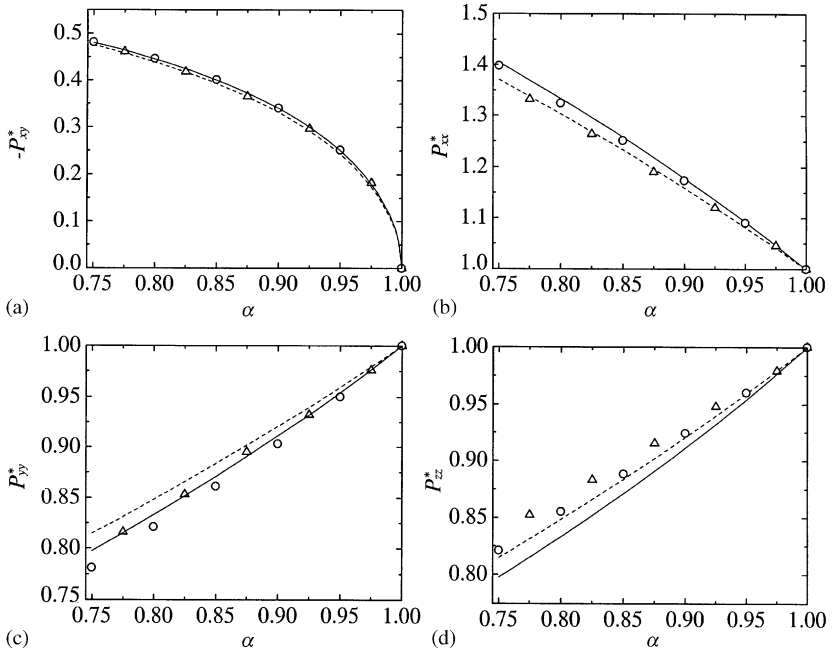

Fig. 7. Plot of the reduced elements of the pressure tensor: (a) $-P^*_{xy} = -P_{xy}/p$, (b) $P^*_{xx} = P_{xx}/p$, (c) $P^*_{yy} = P_{yy}/p$ and (d) $P^*_{zz} = P_{zz}/p$ versus the restitution coefficient α as obtained from simulation (symbols) and the Sonine approximation (lines). We have considered $\mu = m_1/m_2 = 1$, $\delta = n_1/n_2 = 1$, and two different values of the size ratio $w = \sigma_{11}/\sigma_{22}$: $w = 2$ ((—) and ◯), and $w = 1$ ((- - -) and △).

and the parameters of the mixture, namely the mass ratio μ, the concentration ratio δ and the size ratio w. The results clearly indicate that the deviation of the above quantities from their functional forms for elastic collisions is quite important, even for moderate dissipation. In particular, the temperature ratio, which measures the distribution of kinetic energy between both species, is different from unity and presents a complex dependence on the parameters of the problem. This result contrasts with previous results derived for granular mixtures [4–7] where the equality of the partial temperatures in the small inelasticity limit was consistently assumed. However, as the restitution coefficient decreases, the system goes away from equilibrium and consequently, the energy equipartition does not hold. In the same way as in the homogeneous cooling state problem [10,28], the deviations from the energy equipartition can be weak or strong depending on the mechanical differences between the species and the degree of dissipation. On the other hand, the simulation as well as the theoretical results also show that the steady total temperature T^* can be fitted by a linear function of $(1-\alpha^2)^{-1}$ with independence of the values of the parameters of the mixture. This extends previous results derived in the context of simple granular gases by using molecular dynamics [32] or Monte Carlo simulations [19,20]. With respect to the rheological properties, comparison between theory and simulation shows a good quantitative

agreement, especially for the shear stress P_{xy}^*, which is the most relevant element of the pressure tensor in a shearing problem. Although the kinetic theory also predicts normal stresses, the discrepancies between theory and simulation are larger than those found for the temperature ratio or the shear stress.

It is illustrative to make some comparison between the predictions made from our two-temperature theory with those obtained if the differences in the partial temperatures were neglected ($T_1=T_2=T$). For instance, let us consider the mixture $\sigma_{11}=\sigma_{22}$, $n_1=n_2$, and $m_1=10m_2$ with $\alpha=0.75$. In this case, for the xy and yy elements of the pressure tensor, the simulation results are $-P_{xy}^*=0.498$ and $P_{yy}^*=0.723$. Our two-temperature theory predicts $-P_{xy}^*=0.498$ and $P_{yy}^*=0.743$ while the single-temperature theory (assumption made in previous works) gives $-P_{xy}^*=0.456$ and $P_{yy}^*=0.815$. Clearly, inclusion of the two-temperature effects improves the theoretical estimations and makes a significant (quantitative) difference with respect to the predictions of the single-temperature theory.

As a final comment, let us mention that the study made here can in principle be extended in both aspects, kinetic theory and simulations, to the revised Enskog equation in order to assess the influence of finite density on the rheological properties of the mixture. Work along this line is in progress.

Acknowledgements

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Appendix A. Evaluation of the cooling rates

In this appendix the (reduced) cooling rates ζ_i^* are evaluated by using the first Sonine approximation (25). The cooling rate is given by

$$\zeta_i^* = -\frac{2}{3}\pi^{-1/2}\theta_i \sum_j \int d\mathbf{V}_1^*\, V_1^{*2} J_{ij}^*[\mathbf{V}_1^*|f_i^*, f_j^*]\,, \tag{A.1}$$

where $\theta_i = 1/(\gamma_i\mu_{ji})$, $\mathbf{V}_1^* = \mathbf{V}_1/v_0$, $J_{ij}^* = (v_0^2/n_i n\sigma_{12}^2)J_{ij}$, and $f_i^* = (v_0^3/n_i)f_i$. Henceforth, it will be understood that dimensionless quantities will be used and the asterisks will be deleted to simplify the notation. A useful identity for an arbitrary function $h(\mathbf{V}_1)$ is given by

$$\int d\mathbf{V}_1 h(\mathbf{V}_1) J_{ij}[\mathbf{V}_1|f_i, f_j] = x_j \left(\frac{\sigma_{ij}}{\sigma_{12}}\right)^2 \int d\mathbf{V}_1 \int d\mathbf{V}_2\, f_i(\mathbf{V}_1) f_j(\mathbf{V}_2) \times \int d\hat{\boldsymbol{\sigma}}\, \Theta(\hat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})(\hat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})[h(\mathbf{V}_1'') - h(\mathbf{V}_1)]\,, \tag{A.2}$$

with

$$\mathbf{V}_1'' = \mathbf{V}_1 - \mu_{ji}(1+\alpha_{ij})(\hat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})\hat{\boldsymbol{\sigma}}\,. \tag{A.3}$$

This result applies for both $i=j$ and $i\neq j$. Use of this identity in Eq. (A.1) allows the angular integrals to be performed. The result is

$$\zeta_i = (1-\alpha_{ii}^2)\frac{1}{12}\sqrt{\pi}\theta_i x_i \left(\frac{\sigma_{ii}}{\sigma_{12}}\right)^2 \int d\mathbf{V}_1 \int d\mathbf{V}_2\, g_{12}^3 f_i(\mathbf{V}_1) f_i(\mathbf{V}_2)$$

$$+(1-\alpha_{ij}^2)\frac{1}{3}\sqrt{\pi}\theta_i \mu_{ji}^2 x_j \int d\mathbf{V}_1 \int d\mathbf{V}_2\, g_{12}^3 f_i(\mathbf{V}_1) f_j(\mathbf{V}_2)$$

$$+(1+\alpha_{ij})\frac{2}{3}\sqrt{\pi}\theta_i \mu_{ji} x_j \int d\mathbf{V}_1 \int d\mathbf{V}_2\, g_{12}(\mathbf{g}_{12}\cdot\mathbf{G}_{ij}) f_i(\mathbf{V}_1) f_j(\mathbf{V}_2)\,, \tag{A.4}$$

where $\mathbf{G}_{ij}=\mu_{ij}\mathbf{V}_1+\mu_{ji}\mathbf{V}_2$. Now we consider the Sonine approximation (25) for the distributions f_i:

$$f_i(\mathbf{V}_1) \to \left(\frac{\theta_i}{\pi}\right)^{3/2} \mathrm{e}^{-\theta_i V_1^2}\left[1+\theta_i C_{i,k\ell}\left(V_{1,k}V_{1,\ell}-\frac{1}{3}V_1^2\delta_{k\ell}\right)\right]\,. \tag{A.5}$$

Neglecting nonlinear terms in the tensor $C_{i,k\ell}$, the expression (A.4) can be written as

$$\zeta_i = (1-\alpha_{ii}^2)\frac{1}{12}\,\pi^{-5/2}\theta_i^{-1/2} x_i \left(\frac{\sigma_{ii}}{\sigma_{12}}\right)^2 \int d\mathbf{V}_1 \int d\mathbf{V}_2\, g_{12}^3\, \mathrm{e}^{-(V_1^2+V_2^2)}$$

$$+(1-\alpha_{ij}^2)\frac{1}{3}\,\pi^{-5/2}(\theta_i\theta_j)^{3/2}\mu_{ji}^2 x_j\theta_i \int d\mathbf{V}_1 \int d\mathbf{V}_2\, g_{12}^3\, \mathrm{e}^{-(\theta_i V_1^2+\theta_j V_2^2)} + (1+\alpha_{ij})$$

$$\times\frac{2}{3}\,\pi^{-5/2}(\theta_i\theta_j)^{3/2}\mu_{ji} x_j\theta_i \int d\mathbf{V}_1 \int d\mathbf{V}_2\, g_{12}(\mathbf{g}_{12}\cdot\mathbf{G}_{ij})\, \mathrm{e}^{-(\theta_i V_1^2+\theta_j V_2^2)}\,. \tag{A.6}$$

Here, use has been made of the fact the scalar ζ_i^* cannot be coupled to the traceless tensor $C_{i,k\ell}$ so that the only nonzero contribution to the cooling rate comes from the Maxwellian term (first term of the right-hand side of (A.5)) of the distribution function. The first integral of Eq. (A.6) is straightforward and can be done with a change of variables to relative and center of mass variables. The next two integrals are somewhat more complicated and they can be performed by the change of variables

$$\mathbf{x}=\mathbf{V}_1-\mathbf{V}_2, \quad \mathbf{y}=\theta_i\mathbf{V}_1+\theta_j\mathbf{V}_2\,, \tag{A.7}$$

with the Jacobian $(\theta_i+\theta_j)^{-3}$. The integrals can be now easily performed and the final result for ζ_1 is

$$\zeta_1 = \frac{2}{3}\sqrt{2}\left(\frac{\sigma_{11}}{\sigma_{12}}\right)^2 x_1\theta_1^{-1/2}(1-\alpha_{11}^2)$$

$$+\frac{4}{3}\,x_2\mu_{21}\left(\frac{\theta_1+\theta_2}{\theta_1\theta_2}\right)^{1/2}(1+\alpha_{12})\left[2-\mu_{21}(1+\alpha_{12})\frac{\theta_1+\theta_2}{\theta_2}\right]\,. \tag{A.8}$$

The result for ζ_2 is obtained from Eq. (A.8) by interchanging 1 and 2.

Appendix B. Evaluation of the collisional moments

In reduced units, the collisional moments $A_{k\ell}^{ij}$ are given by

$$A_{k\ell}^{ij} = \frac{m_i v_0^2}{T}\,\pi^{-1/2}\int d\mathbf{V}_1 V_{1,k} V_{1,\ell} J_{ij}[\mathbf{V}_1|f_i,f_j]$$

$$= \frac{m_i v_0^2}{T}\,x_j \pi^{-1/2}\left(\frac{\sigma_{ij}}{\sigma_{12}}\right)^2 \int d\mathbf{V}_1 \int d\mathbf{V}_2 f_i(\mathbf{V}_1) f_j(\mathbf{V}_2) \int d\hat{\boldsymbol{\sigma}}\,\Theta(\hat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})$$

$$\times(\hat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})\left(V_{1,k}'' V_{1,\ell}'' - V_{1,k} V_{1,\ell}\right)\,, \tag{B.1}$$

where the identity (A.2) has been used. Substitution of (A.3) into Eq. (B.1) allows the angular integral to be performed with the result

$$A_{k\ell}^{ij} = -\frac{\sqrt{\pi}}{2}\frac{m_i v_0^2}{T}\mu_{ji} x_j \left(\frac{\sigma_{ij}}{\sigma_{12}}\right)^2 (1+\alpha_{ij}) \int d\mathbf{V}_1 \int d\mathbf{V}_2 f_i(\mathbf{V}_1) f_j(\mathbf{V}_2)$$

$$\times\left[g_{12}(G_{ij,k} g_{12,\ell} + G_{ij,\ell} g_{12,k}) + \frac{\mu_{ji}}{2}(3-\alpha_{ij}) g_{12} g_{12,k} g_{12,\ell}\right.$$

$$\left. - \frac{\mu_{ji}}{6}(1+\alpha_{ij}) g_{12}^3 \delta_{k\ell}\right]\,, \tag{B.2}$$

where $g_{12,k} = V_{1,k} - V_{2,k}$ and $G_{ij,k} = \mu_{ij} V_{1,k} + \mu_{ji} V_{2,k}$. To perform the integral we use the Sonine approximation of f_i and the change of variables (A.7). When one neglects again nonlinear terms in the tensor C_i, the collisional moment $A_{k\ell}^{ij}$ becomes

$$A_{k\ell}^{ij} = -\frac{1}{2}\pi^{-5/2}\frac{m_i v_0^2}{T}\mu_{ji} x_j \left(\frac{\sigma_{ij}}{\sigma_{12}}\right)^2 (1+\alpha_{ij}) \frac{(\theta_i\theta_j)^{3/2}}{(\theta_i+\theta_j)^3} \int d\mathbf{x} \int d\mathbf{y}\, e^{-(b_{ij}x^2 + d_{ij}y^2)}$$

$$\times[1 + \theta_i(\theta_i+\theta_j)^{-2}\mathsf{C}_i : (\mathbf{y}+\theta_j\mathbf{x})(\mathbf{y}+\theta_j\mathbf{x})$$

$$+ \theta_j(\theta_i+\theta_j)^{-2}\mathsf{C}_j : (\mathbf{y}-\theta_i\mathbf{x})(\mathbf{y}-\theta_i\mathbf{x})]$$

$$\times\left[(\theta_i+\theta_j)^{-1} x(x_k y_\ell + x_\ell y_k) + \lambda_{ij} x x_k x_\ell - \frac{\mu_{ji}}{6}(1+\alpha_{ij}) x^3 \delta_{k\ell}\right]\,, \tag{B.3}$$

where

$$b_{ij} = \theta_i\theta_j(\theta_i+\theta_j)^{-1}\,, \tag{B.4}$$

$$d_{ij} = (\theta_i+\theta_j)^{-1}\,, \tag{B.5}$$

$$\lambda_{ij} = 2\,\frac{\mu_{ij}\theta_j - \mu_{ji}\theta_i}{\theta_i+\theta_j} + \frac{\mu_{ji}}{2}(3-\alpha_{ij})\,. \tag{B.6}$$

The corresponding integrals can be now easily performed and, after some algebra, the final result is

$$A_{k\ell}^{ij} = \frac{2}{3}\frac{m_i v_0^2}{T}\mu_{ji}x_j\left(\frac{\sigma_{ij}}{\sigma_{12}}\right)^2(1+\alpha_{ij})\left(\frac{\theta_i+\theta_j}{\theta_i\theta_j}\right)^{3/2}$$
$$\times\left\{[\tfrac{1}{5}\lambda_{ij}+\tfrac{1}{2}\mu_{ji}(1+\alpha_{ij})]\delta_{k\ell}-2\frac{\theta_i\theta_j}{(\theta_i+\theta_j)^2}\left[\left(1+\tfrac{3}{5}\lambda_{ij}\frac{\theta_i+\theta_j}{\theta_i}\right)\gamma_i^{-1}P_{i,k\ell}\right.\right.$$
$$\left.\left.-\left(1-\tfrac{3}{5}\lambda_{ij}\frac{\theta_i+\theta_j}{\theta_j}\right)\gamma_j^{-1}P_{j,k\ell}\right]\right\}. \tag{B.7}$$

From this general expression one can get the collisional moments $A_{k\ell}^{11}$, $A_{k\ell}^{12}$, $A_{k\ell}^{22}$, and $A_{k\ell}^{21}$. In particular,

$$A_{k\ell}^{11} = F_{11}\delta_{k\ell}+G_{11}P_{1,k\ell}\,, \tag{B.8}$$

$$A_{k\ell}^{12} = F_{12}\delta_{k\ell}+G_{12}P_{1,k\ell}+H_{12}P_{2,k\ell}\,, \tag{B.9}$$

where

$$F_{11} = \frac{4}{15}\sqrt{2}\mu_{21}^{-1}x_1\left(\frac{\sigma_{11}}{\sigma_{12}}\right)^2\theta_1^{-3/2}(1+\alpha_{11})(2+\alpha_{11})\,, \tag{B.10}$$

$$G_{11} = -\frac{2}{5}\sqrt{2}x_1\left(\frac{\sigma_{11}}{\sigma_{12}}\right)^2\theta_1^{-1/2}(1+\alpha_{11})(3-\alpha_{11})\,, \tag{B.11}$$

$$F_{12} = \frac{4}{3}x_2(1+\alpha_{12})\left(\frac{\theta_1+\theta_2}{\theta_1\theta_2}\right)^{3/2}[\tfrac{1}{5}\lambda_{12}+\tfrac{1}{2}\mu_{21}(1+\alpha_{12})]\,, \tag{B.12}$$

$$G_{12} = -\frac{8}{3}x_2\mu_{21}(1+\alpha_{12})\left(\frac{\theta_1}{\theta_2(\theta_1+\theta_2)}\right)^{1/2}\left(1+\frac{3}{5}\lambda_{12}\frac{\theta_1+\theta_2}{\theta_1}\right), \tag{B.13}$$

$$H_{12} = \frac{8}{3}x_2\mu_{12}(1+\alpha_{12})\left(\frac{\theta_2}{\theta_1(\theta_1+\theta_2)}\right)^{1/2}\left(1-\frac{3}{5}\lambda_{12}\frac{\theta_1+\theta_2}{\theta_2}\right). \tag{B.14}$$

The corresponding expressions for F_{22}, G_{22}, F_{21}, G_{21}, and H_{21} can be easily inferred from Eqs. (B.10)–(B.14) by just making the changes $1\leftrightarrow 2$. From Eqs. (B.8)–(B.14) and (A.8), it is easy to prove the identity

$$-\gamma_1\zeta_1 = F_{11}+F_{12}+(G_{11}+G_{12})\gamma_1+H_{12}\gamma_2\,, \tag{B.15}$$

which is in fact required by the partial energy conservation equation (22) to support the solution found for the simple shear flow problem. In the case of mechanically

equivalent particles, the expression of the collisional moments $A_{k\ell}^{ij}$ are

$$A_{k\ell}^{11} + A_{k\ell}^{12} = \frac{4}{15}(1+\alpha)\left[(2+\alpha)\delta_{k\ell} - \frac{3}{2}(3-\alpha)P_{k\ell}\right] . \tag{B.16}$$

When $\alpha = 1$, Eq. (B.16) reduces to the results derived from the Boltzmann equation in the first Sonine approximation.

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