

# Energy Nonequpartition in a Sheared Granular Mixture

JOSÉ MARÍA MONTANERO<sup>a,\*</sup> and VICENTE GARZÓ<sup>b</sup>

<sup>a</sup>Departamento de Electrónica e Ingeniería Electromecánica, Universidad de Extremadura, E-06071 Badajoz, Spain; <sup>b</sup>Departamento de Física, Universidad de Extremadura, E-06071 Badajoz, Spain

(Received July 2002; In final form September 2002)

The kinetic granular temperatures of a binary granular mixture in simple shear flow are calculated by means of the Direct Simulation Monte Carlo method. The results show that the temperature ratio is clearly different from unity (as may be expected since the system is out of equilibrium) and strongly depends on the restitution coefficients as well as on the parameters of the mixture. The influence of the temperature differences on the rheological properties is also discussed. The results are compared with the theoretical predictions obtained from the Boltzmann kinetic theory by using a Sonine polynomial expansion. The comparison shows an excellent agreement over the range of parameters investigated.

**Keywords:** Monte Carlo simulation; Sheared granular mixture; Kinetic theory; Sonine polynomial expansion

**PACS number(s):** 45.70.Mg; 05.20.Dd; 51.10.+y; 47.50.+d

## INTRODUCTION

Although experimental and theoretical studies on granular media have been mainly focused on assemblies of identical particles, there appears to be a recent growing interest among both theorists and experimentalists in the more complicated case of polydisperse systems. In this case, several kinetic theory studies in the freely cooling [1,2] and thermostatted steady [3] states have shown that the kinetic temperatures of each species are different. This violation of energy equipartition has been subsequently confirmed in experiments of vibrated granular mixtures [4,5] and in recent molecular dynamics (MD) simulations [6] of the homogeneous cooling state. When the system is sheared, a similar

result has been found by Clelland and Hrenya [7] from MD simulations of a binary-sized mixture of inelastic, smooth hard disks engaged in rapid shear flow. Their results were compared with previous kinetic theory calculations [8,9] based on the assumption of equipartition of granular energy. As Clelland and Hrenya conclude [7], although this equipartition-of-energy assumption does not appear to have a great negative impact on the ability of those earliest theories to predict the stress tensor in simple shear flow, a *multi-temperature* theory must be more appropriate.

The goal of this paper is to analyze the dependence of the temperature ratio  $\gamma \equiv T_1/T_2$  on particle properties as well as on compositional parameters of a granular binary mixture subjected to the simple shear flow. Our motivation is two-fold. First, the calculation of  $\gamma$  allows one to assess the magnitude of the equipartition violation and its dependence on the parameters of the system. Second, given that in general  $\gamma \neq 1$ , we want also to evaluate what is the influence of temperature differences on the rheological properties of the mixture. As will be shown later, the consequences of the two-temperature effect for the shear and normal stresses are significant, especially for strong dissipation, and so energy nonequpartition must be taken into account in studying transport properties in granular mixtures [10].

Due to the complexity of the general problem, here we will restrict ourselves to the low-density regime. In this context, and from a numerical point of view, the Direct Simulation Monte Carlo (DSMC) method [11] is the most convenient algorithm to study non-equilibrium phenomena. It was devised to mimic the dynamics involved in the Boltzmann collision term.

\*Corresponding author. E-mail: jmm@unex.es

The extension of the DSMC method to deal with inelastic collisions is straightforward [2,12–14], 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 MD simulations. Also, the restriction to this homogeneous state prevents us from analyzing the possible instability of simple shear flow or the formation of clusters or microstructures. A previous study of the dependence of the temperature ratio on the parameters of the mixture was carried out in Ref. [14] for a three-dimensional system. In this paper, we extend such analysis for a general  $d$ -dimensional fluid as well as make a comparison with other theories in the case of hard disks. In addition, apart from computing the temperature ratio, we are also interested in evaluating the elements of the stress tensor in order to test the accuracy of our two-temperature description with respect to previous single-temperature theories.

In the context of kinetic theory, the only primary attempts to include temperature differences in dense granular mixtures were put forward by Jenkins and Mancini [15] and more recently by Huilin *et al.* [16,17]. These theories are applicable to a general flow field. However, both works are phenomenological with no attempt to solve the kinetic equation. Instead, they assume that the velocity distribution functions are local Maxwellians. This can be reasonable to estimate the dense gas collisional transfer contributions to the fluxes, but not to compute their kinetic contributions. As shown in the following, the low-density results of the Jenkins and Mancini theory [15] present important discrepancies with computer simulations and consequently, this theory does not estimate well the kinetic part of the stress tensor.

In this paper, the simulation results are compared with those calculated from the nonlinear Boltzmann equations for the velocity distribution functions for the two species. This set of equations is first analytically solved by using a Sonine polynomial approximation, explicitly getting the temperature ratio as function of the mass ratio, size ratio, composition and restitution coefficients. Then, to check the reliability of our theoretical predictions, we compare them with those obtained from Monte Carlo simulations for hard disks ( $d = 2$ ) over a wide range of parameter space. As happens in the three-dimensional case [14], our theory compares quite well with DSMC results.

The plan of the paper is as follows. In the second section we describe the simple flow problem and give a brief survey of the Sonine approximation used. The computer simulation method employed to

numerically solve the Boltzmann equation for a dissipative fluid under shear flow is described in the third section. The paper is closed in the fourth section with a careful comparison between theory and simulation as well as with a brief discussion on the results obtained.

## SIMPLE SHEAR FLOW

Let us consider a granular binary mixture composed by smooth inelastic disks or spheres of masses  $m_1$  and  $m_2$  and diameters  $\sigma_1$  and  $\sigma_2$ . Collisions between particles are inelastic and characterized by three constant (independent) restitution coefficients  $\alpha_{11}$ ,  $\alpha_{22}$  and  $\alpha_{12} = \alpha_{21}$ , where  $\alpha_{ij} \leq 1$  refers to the restitution coefficient for collisions between particles of species  $i$  and  $j$ . The mixture is under simple shear flow, namely, a macroscopic state with a constant linear velocity profile  $\mathbf{U} = \mathbf{a} \cdot \mathbf{r}$ , where  $a_{kl} = a \delta_{kx} \delta_{ly}$ ,  $a$  being the constant shear rate. In addition, the partial densities  $n_i$  and the (global) granular temperature  $T$  are uniform. The simple shear flow state has been extensively studied for molecular fluids as a prototype problem to analyze nonlinear transport properties [18]. Nevertheless, the nature of this state is quite different in the case of granular fluids. While for elastic fluids the temperature grows monotonically in time due to viscous heating, a steady state is possible for granular media when the effect of viscosity is exactly compensated by the collisional cooling. In this case, the system reaches a steady state and the temperature achieves a constant value. This steady state is what we want to analyze here.

From a microscopic point of view, the simple shear flow problem becomes spatially uniform in the local Lagrangian frame moving with the flow velocity  $\mathbf{U}$ . In this frame, the velocity distribution functions become uniform:  $f_i(\mathbf{r}, \mathbf{v}) \rightarrow f_i(\mathbf{V})$ , where  $\mathbf{V} = \mathbf{v} - \mathbf{U}$  is the peculiar velocity. Under these conditions, the set of Boltzmann kinetic equations read [14]

$$-aV_y \frac{\partial}{\partial V_x} f_i(\mathbf{V}) = \sum_j J_{ij}[\mathbf{V}|f_i, f_j], \quad (1)$$

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

$$J_{ij}[\mathbf{V}_1|f_i, f_j] = \sigma_{ij}^{d-1} \int d\mathbf{V}_2 \int d\hat{\mathbf{g}} \Theta(\hat{\mathbf{g}} \cdot \mathbf{g}_{12}) (\hat{\mathbf{g}} \cdot \mathbf{g}_{12}) \\ \times \left[ \alpha_{ij}^{-2} f_i(\mathbf{V}'_1) f_j(\mathbf{V}'_2) - f_i(\mathbf{V}_1) f_j(\mathbf{V}_2) \right]. \quad (2)$$

Here,  $d$  is the dimensionality of the system,  $\sigma_{ij} = (\sigma_i + \sigma_j)/2$ ,  $\hat{\mathbf{g}}$  is a unit vector along their line of centers,  $\Theta$  is the Heaviside step

function and  $\mathbf{g}_{12} = \mathbf{V}_1 - \mathbf{V}_2$ . In addition, 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:

$$\begin{aligned}\mathbf{V}'_1 &= \mathbf{V}_1 - \mu_{ji} \left(1 + \alpha_{ij}^{-1}\right) (\hat{\mathbf{c}} \cdot \mathbf{g}_{12}) \hat{\mathbf{c}}, \\ \mathbf{V}'_2 &= \mathbf{V}_2 + \mu_{ij} \left(1 + \alpha_{ij}^{-1}\right) (\hat{\mathbf{c}} \cdot \mathbf{g}_{12}) \hat{\mathbf{c}},\end{aligned}\quad (3)$$

where  $\mu_{ij} = m_i/(m_i + m_j)$ .

Our study is mainly focused on the evaluation of the partial temperatures  $T_i$ , which measure the mean kinetic energy of each species. In terms of the distributions  $f_i$ , they are defined as

$$\frac{d}{2} n_i T_i = \int d\mathbf{V} \frac{1}{2} m_i V^2 f_i. \quad (4)$$

The temperature of the mixture is  $T = x_1 T_1 + x_2 T_2$ , where  $x_i = n_i/(n_1 + n_2)$  is the mole fraction of species  $i$ . The balance equation of the granular temperature for species  $i$  can be obtained by multiplying the Boltzmann equation (1) by  $m_i V^2$  and integrating over  $\mathbf{V}$ . The result is

$$a P_{i,xy} + \frac{d}{2} \xi_i p_i = 0, \quad (5)$$

where  $p_i = n_i T_i$ ,

$$\mathbf{P}_i = m_i \int d\mathbf{V} \mathbf{V} \mathbf{V} f_i(\mathbf{V}), \quad (6)$$

is the partial pressure tensor of the species  $i$  and  $\xi_i = \sum_j \zeta_{ij}$  is the cooling rate associated with the partial temperature  $T_i$ , where

$$\zeta_{ij} = -\frac{1}{dn_i T_i} \int d\mathbf{V} m_i V^2 J_{ij}[\mathbf{V}|f_i, f_j]. \quad (7)$$

The total cooling rate  $\zeta$  corresponding to the granular temperature  $T$  is defined as

$$\zeta = \frac{1}{T} \sum_{i=1}^2 x_i T_i \zeta_i. \quad (8)$$

The total pressure tensor of the mixture is

$$\mathbf{P} = \sum_{i=1}^2 \mathbf{P}_i. \quad (9)$$

According to Eq. (5), in the steady state the temperature ratio  $\gamma \equiv T_1/T_2$  is given by the relation

$$\gamma = \frac{x_2 \zeta_2 P_{1,xy}}{x_1 \zeta_1 P_{2,xy}}. \quad (10)$$

Thus, to get  $\gamma$  one needs to determine the cooling rates  $\zeta_i$  and the  $xy$  element of the partial pressure tensors  $\mathbf{P}_i$ . An equation for the elements of  $\mathbf{P}_i$  follows immediately from the definition (6) and

the Boltzmann equation (1):

$$a_{km} P_{i,ml} + a_{lm} P_{i,mk} = \sum_{j=1}^2 A_{ij,kl}, \quad (11)$$

where we have introduced the collisional moments  $\mathbf{A}_{ij}$  as

$$\mathbf{A}_{ij} = m_i \int d\mathbf{V} \mathbf{V} \mathbf{V} J_{ij}[\mathbf{V}|f_i, f_j]. \quad (12)$$

The determination of  $\mathbf{P}_i$  is a closed problem provided the moments  $\mathbf{A}_{ij}$  are explicitly known. This requires the knowledge of the velocity distribution functions  $f_i$ , which is quite an intricate problem, even in the elastic case. A useful way to estimate  $\zeta_i$  and  $\mathbf{A}_{ij}$  is to expand  $f_i$  in Sonine polynomials. This approach is similar to the usual moment method for solving kinetic equations in the elastic case where the leading order truncation is known to be a good approximation. In the case of shear flow, we take the leading Sonine approximation:

$$f_i(\mathbf{V}) \rightarrow f_{i,M}(\mathbf{V}) [1 + \mathbf{C}_i : \mathbf{D}_i(\mathbf{V})/2T_i] \quad (13)$$

where

$$\mathbf{C}_i = \frac{\mathbf{P}_i}{p_i} - \mathbb{1}, \quad \mathbf{D}_i(\mathbf{V}) = m_i \left( \mathbf{V} \mathbf{V} - \frac{V^2}{d} \mathbb{1} \right). \quad (14)$$

Here,  $\mathbb{1}$  is the  $d \times d$  unit tensor and  $f_{i,M}$  is a Maxwellian distribution at the temperature of the species  $i$ , i.e.

$$f_{i,M}(\mathbf{V}) = n_i \left( \frac{m_i}{2\pi T_i} \right)^{d/2} \exp \left( -\frac{m_i V^2}{2T_i} \right). \quad (15)$$

With this approximation, the integrals appearing in the expressions of the cooling rates  $\zeta_{ij}$  and the collisional moments  $\mathbf{A}_{ij}$  can be explicitly evaluated. Retaining only linear terms in  $\mathbf{C}_i$  and after a lengthy calculation, one gets [19]

$$\begin{aligned}\zeta_{ij} &= \frac{2\pi^{(d-1)/2}}{d\Gamma(d/2)} n_i \mu_{ji} \sigma_{ij}^{d-1} v_0 \left( \frac{\theta_i + \theta_j}{\theta_i \theta_j} \right)^{1/2} (1 + \alpha_{ij}) \\ &\quad \times \left[ 2 - \mu_{ji} (1 + \alpha_{ij}) \frac{\theta_i + \theta_j}{\theta_j} \right],\end{aligned}\quad (16)$$

$$\begin{aligned}\mathbf{A}_{ij} &= -\frac{\pi^{(d-1)/2}}{d\Gamma(d/2)} m_i n_i n_j \mu_{ji} \sigma_{ij}^{d-1} v_0^3 \left( \frac{\theta_i + \theta_j}{\theta_i \theta_j} \right)^{3/2} (1 + \alpha_{ij}) \\ &\quad \times \left\{ \left[ \lambda_{ij} - \frac{d}{d+3} \mu_{ji} (1 + \alpha_{ij}) \right] \mathbb{1} \right. \\ &\quad \left. + 2 \frac{\theta_i \theta_j}{(\theta_i + \theta_j)^2} \left[ \left( 1 + \frac{d+3}{2(d+2)} \frac{\theta_i + \theta_j}{\theta_i} \lambda_{ij} \right) \mathbf{C}_i \right. \right. \\ &\quad \left. \left. - \left( 1 - \frac{d+3}{2(d+2)} \frac{\theta_i + \theta_j}{\theta_j} \lambda_{ij} \right) \mathbf{C}_j \right] \right\}. \quad (17)\end{aligned}$$

In these expressions,  $v_0 = \sqrt{2T(m_1 + m_2)/m_1 m_2}$  is a thermal velocity defined in terms of the temperature

of the mixture  $T$ , and

$$\theta_1 = \frac{1 + x_1(\gamma - 1)}{\mu_{21}\gamma}, \quad \theta_2 = \frac{1 + x_1(\gamma - 1)}{\mu_{12}}, \quad (18)$$

$$\lambda_{ij} = 2 \frac{\mu_{ij}\theta_j - \mu_{ji}\theta_i}{\theta_i + \theta_j} + \frac{\mu_{ji}}{d+3} (2d+3 - 3\alpha_{ij}). \quad (19)$$

Equations (16) and (17) extend previous expressions [14] obtained in the three-dimensional case. The approximation (17) allows one to solve the set of equations (11) and express  $\mathbf{P}_i$  as a function of  $\gamma$ , while the approximation (16) gives the cooling rates  $\zeta_i$ . When all these expressions are used in Eq. (10), one gets a closed equation for the temperature ratio  $\gamma$ , that can be solved numerically. Once the temperature ratio is known, the elements of the pressure tensor  $\mathbf{P}$  can be explicitly obtained.

### DIRECT SIMULATION MONTE CARLO METHOD

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:

$$f_i(\mathbf{V}, t) \rightarrow n_i \frac{1}{N_i} \sum_{k=1}^{N_i} \delta(\mathbf{V} - \mathbf{V}_k(t)). \quad (20)$$

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:

$$f_i(\mathbf{V}, 0) = n_i \pi^{-d/2} V_{0i}^{-d} \exp(-\mathbf{V}^2/V_{0i}^2(0)), \quad (21)$$

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  $\Delta t$  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  $\mathbf{F}_i = -m_i \mathbf{a} \cdot \mathbf{V}$ . This force is represented by the terms on the left-hand side of Eq. (1). Thus, the free motion stage consists of making  $\mathbf{V}_k \rightarrow \mathbf{V}_k - \mathbf{a} \cdot \mathbf{V}_k \Delta t$ . 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  $(1/2)N_i \omega_{\max}^{(ij)} \Delta t$  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  $\ell$  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  $\hat{\mathbf{g}}_{k\ell}$  is chosen at random with equiprobability; (2) the collision between particles  $k$  and  $\ell$  is accepted with a probability equal to  $\Theta(\mathbf{g}_{k\ell} \cdot \hat{\mathbf{g}}_{k\ell}) \omega_{k\ell}^{(ij)} / \omega_{\max}^{(ij)}$ , where  $\mathbf{g}_{k\ell} = \mathbf{V}_k - \mathbf{V}_\ell$  and  $\omega_{k\ell}^{(ij)} = 2^{d-1} \tilde{\sigma}_{ij}^2 n_j |\mathbf{g}_{k\ell} \cdot \hat{\mathbf{g}}_{k\ell}|$ ,  $\tilde{\sigma}_{ij}$  being the total cross-section for collisions  $i-j$ ; (3) if the collision is accepted, postcollisional velocities are assigned to both particles according to the scattering rules:

$$\mathbf{V}_k \rightarrow \mathbf{V}_k - \mu_{ji}(1 + \alpha_{ij})(\mathbf{g}_{k\ell} \cdot \hat{\mathbf{g}}_{k\ell}) \hat{\mathbf{g}}_{k\ell}, \quad (22)$$

$$\mathbf{V}_\ell \rightarrow \mathbf{V}_\ell + \mu_{ij}(1 + \alpha_{ij})(\mathbf{g}_{k\ell} \cdot \hat{\mathbf{g}}_{k\ell}) \hat{\mathbf{g}}_{k\ell}. \quad (23)$$

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  $\mathbf{P}$  and the partial temperatures  $T_i$ . They are given as

$$\mathbf{P} = \sum_{i=1}^2 \frac{m_i n_i}{N_i} \sum_{k=1}^{N_i} \mathbf{V}_k \mathbf{V}_k, \quad (24)$$

$$T_i = \frac{m_i}{dN_i} \sum_{k=1}^{N_i} \mathbf{V}_k^2. \quad (25)$$

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  $\lambda_{11} = (\sqrt{2} n_1 \sigma_1^2)^{-1}$  is the mean free path for collisions  $1-1$ .

As mentioned above, in the simulations the initial velocity distribution function is that of local equilibrium (21). After an initial transient period, the system reaches the steady state. The values obtained for the reduced quantities  $\gamma$  and  $\mathbf{P}^* = \mathbf{P}/nT$  in this state are independent of the initial preparation of the system, and only depend on the values of the restitution coefficients and the ratios of mass, concentration and sizes. We will mainly focus on the influence of the restitution coefficients and the parameters of the mixture on the (steady) temperature ratio.

### RESULTS AND DISCUSSION

A full presentation of the results is not possible because of the complexity of the parameter space:  $\alpha_{11}$ ,  $\alpha_{22}$ ,  $\alpha_{12}$ ,  $m_1/m_2$ ,  $x_1$  and  $\sigma_1/\sigma_2$ . As in Ref. [7], we assume for simplicity that the spheres or disks are made of the same material, and thereby

$\alpha_{11} = \alpha_{22} = \alpha_{12} \equiv \alpha$  and  $m_1/m_2 = (\sigma_1/\sigma_2)^d$ . This reduces the parameter space to  $\alpha$ ,  $x_1$  and  $\sigma_1/\sigma_2$ . As expected, our results show that in general the kinetic temperatures of the mixture are different ( $\gamma \neq 1$ ). There are only two trivial exceptions: the elastic case ( $\alpha = 1$ ) and the case of mechanically equivalent particles ( $m_1 = m_2$ ,  $\sigma_1 = \sigma_2$ ). Beyond these cases, the dependence of  $\gamma$  on the parameters of the problem is quite intricate. As an illustration, we plot the simulation results and the theoretical predictions for the temperature ratio  $T_1/T_2$  versus the diameter ratio  $\sigma_1/\sigma_2$  for  $x_1 = 1/3$  (Fig. 1) and  $x_1 = 1/2$  (Fig. 2) for three different values of  $\alpha$ :  $\alpha = 0.95$ ,  $\alpha = 0.9$  and  $\alpha = 0.8$ . We have considered the two-dimensional case ( $d = 2$ ). Also, for comparison we show the kinetic theory predictions of Jenkins and Mancini [15] particularized to the low-density regime.

It is apparent that an excellent agreement between Monte Carlo simulations (symbols) and our theory is found over the entire range of values of size and mass ratios considered. Although the solid fractions considered by Clelland and Hrenya [7] prevent us from making a quantitative comparison between our theory and their MD simulations, we observe that the behavior of  $\gamma$  in dilute systems is qualitatively similar to that found in Ref. [7] for a finite-density systems. Thus, for instance, at a given value of  $\alpha$  the granular energy of the larger particle (say for instance, species 1) increases relative to that of the smaller particle as the size ratio  $\sigma_1/\sigma_2$  increases. Both Monte Carlo simulation and theory show that the temperature ratio presents a strong dependence on the restitution coefficient. With respect to the influence of composition, comparison of Figs. 1 and 2 indicates that  $\gamma$  exhibits a very weak dependence on the mole fraction  $x_1$ . This behavior has been also found in recent experiments [4,5] carried out on binary vibrated granular gases and in MD simulations of the free cooling case. [6] We also

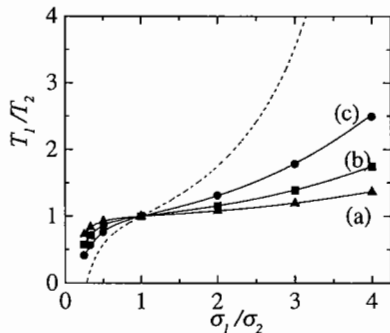


FIGURE 1 Plot of the temperature ratio  $T_1/T_2$  as a function of the size ratio  $(\sigma_1/\sigma_2)^2 = m_1/m_2$  for a two-dimensional system in the case  $x_1 = 1/3$  and three different values of the restitution coefficient  $\alpha$ : (a)  $\alpha = 0.95$ , (b)  $\alpha = 0.9$  and (c)  $\alpha = 0.8$ . The solid lines are the theoretical predictions while the symbols refer to the Monte Carlo simulation results. The dashed line corresponds to the prediction given by the theory of Jenkins and Mancini [15] in the case  $\alpha = 0.8$ .

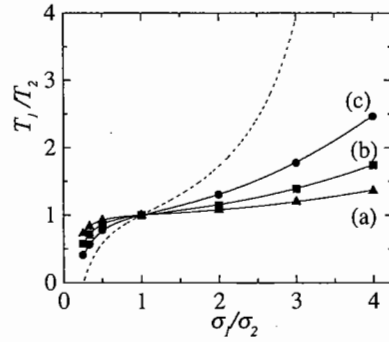


FIGURE 2 Plot of the temperature ratio  $T_1/T_2$  as a function of the size ratio  $(\sigma_1/\sigma_2)^2 = m_1/m_2$  for a two-dimensional system in the case  $x_1 = 1/2$  and three different values of the restitution coefficient  $\alpha$ : (a)  $\alpha = 0.95$ , (b)  $\alpha = 0.9$  and (c)  $\alpha = 0.8$ . The solid lines are the theoretical predictions while the symbols refer to the Monte Carlo simulation results. The dashed line corresponds to the prediction given by the theory of Jenkins and Mancini [15] in the case  $\alpha = 0.8$ .

see that all the above trends are qualitatively reproduced by the theory of Jenkins and Mancini [15] (which is restricted to nearly elastic disks), although they are, however, strongly exaggerated. This is basically due to the fact that the theory of Jenkins and Mancini is especially targeted to dense systems where the collisional transport effects are more important than the kinetic ones.

An interesting point is to assess the influence of the temperature differences on the rheological properties of the mixture. Although the comparison carried out in Ref. [7] between previous theories (based on a single temperature) and simulation shows a qualitative good agreement at the level of the shear stresses, one expects that the new contributions coming from the energy difference leads to an improvement over previous theoretical predictions. In Fig. 3, we plot the dimensionless stresses  $-P_{xy}^*$  and  $P_{yy}^*$  versus the restitution coefficient in the case  $x_1 = 1/2$  and  $m_1/m_2 = (\sigma_1/\sigma_2)^2 = 10$ . Also shown in this Fig. 3 is the result which would be obtained if the differences in the partial temperatures were

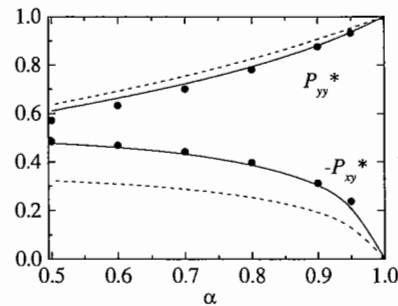


FIGURE 3 Plot of the reduced elements of the pressure tensor  $P_{yy}^* = P_{yy}/nT$  and  $-P_{xy}^* = -P_{xy}/nT$  as a function of the restitution coefficient  $\alpha$  for a two-dimensional system in the case  $(\sigma_1/\sigma_2)^2 = m_1/m_2 = 10$ ,  $x_1 = 1/2$ . The solid lines are the theoretical predictions while the symbols refer to the Monte Carlo simulation results. The dashed lines correspond to the theoretical results by assuming the equality of the partial temperatures  $T_1/T_2 = 1$ .

neglected [i.e.  $\theta_i = \mu_{ji}^{-1}$  in Eqs. (16) and (17)]. In general, inclusion of the two-temperature effects represents a significant improvement of the theory, especially in the case of the shear stress  $P_{xy}^*$ , which is the most relevant rheological property in a sheared flow problem. This justifies the use of a two-temperature description to capture the dependence of stresses on dissipation.

In summary, we have calculated the temperature ratio of a sheared granular mixture by means of the Monte Carlo simulation method. As was also found in recent MD simulations [7], our results show that the temperature ratio strongly depends on dissipation and the mechanical parameters of the mixture, especially on the ratios of mass and size. In addition, the effect of temperature differences on rheology is important, especially in the case of the shear stress. The simulation results have been compared with those obtained analytically from the nonlinear Boltzmann equations by using a first-Sonine polynomial approximation. The accuracy of the theoretical predictions have been confirmed showing that the inclusion of the temperature ratio in the calculations leads to an improvement with respect to the predictions made from a single-temperature theory.

#### Acknowledgements

V. Garzó acknowledges partial support from the Ministerio de Ciencia y Tecnología (Spain) through Grant No. BFM2001-0718.

#### References

- [1] Garzó, V. and Dufty, J.W. (1999) "Homogeneous cooling state for a granular mixture", *Phys. Rev. E*, **60**, 5706.

- [2] Montanero, J.M. and Garzó, V. (2002) "Monte Carlo simulation of the homogeneous cooling state for a granular mixture", *Granular Matter* **4**, 17.
- [3] Barrat, A. and Trizac, E. (2002) "Lack of energy equipartition in homogeneous heated binary granular mixtures", *Granular Matter* **4**, 57.
- [4] Wildman, R.D. and Parker, D.J. (2002) "Coexistence of two granular temperatures in binary vibrofluidized beds", *Phys. Rev. Lett.* **88**, 064301.
- [5] Feitosa, K. and Menon, N. (2002) "Breakdown of energy equipartition in a 2D binary vibrated granular gas", *Phys. Rev. Lett.* **88**, 198301.
- [6] Dahl, S.R., Hrenya, C.M., Garzó, V. and Dufty, J.W. *Phys. Rev. E* **66** (2002), 041301 and cond-mat/0205413.
- [7] Clelland, R. and Hrenya, C. (2002) "Simulations of a binary-sized mixture of inelastic grains in rapid shear flow", *Phys. Rev. E* **65**, 031301.
- [8] Arnarson, B. and Willits, J.T. (1998) "Thermal diffusion in binary mixtures of smooth, nearly elastic spheres with and without gravity", *Phys. Fluids* **10**, 1324.
- [9] Willits, J.T. and Arnarson, B. (1999) "Kinetic theory of a binary mixture of nearly elastic disks", *Phys. Fluids* **11**, 3116.
- [10] Garzó, V. and Dufty, J.W. (2002), *Phys. Fluids* **14**, 1476.
- [11] Bird, G. (1994) *Molecular Gas Dynamics and the Direct Simulation of Gas Flows* (Clarendon Press, Oxford).
- [12] Montanero, J.M., Garzó, V., Santos, A. and Brey, J.J. (1999) "Kinetic theory of simple granular shear flows of smooth hard spheres", *J. Fluid Mech.* **389**, 391.
- [13] Frezzotti, A. (2000) "Monte Carlo simulation of the uniform shear flow in a dense rough sphere fluid", *Phys. A* **278**, 161.
- [14] Montanero, J.M. and Garzó, V. (2002) "Rheological properties in a low-density granular mixture", *Phys. A* **310**, 17.
- [15] Jenkins, J.T. and Mancini, F. (1987) "Balance laws and constitutive relation for plane flows of a dense, binary mixture of smooth, nearly elastic, circular disks", *J. Appl. Mech.* **54**, 27.
- [16] Huilin, L., Wenti, L., Rushan, B., Lidan, Y. and Gidaspow, D. (2000) "Kinetic theory of fluidized binary granular mixtures with unequal granular temperature", *Phys. A* **284**, 265.
- [17] Huilin, L., Gidaspow, D. and Manger, E. (2001) "Kinetic theory of fluidized binary granular mixtures", *Phys. Rev. E* **64**, 061301.
- [18] Evans, D.J. and Morriss, G.P. (1990) *Statistical Mechanics of Nonequilibrium Liquids* (Academic Press, London).
- [19] Garzó, V. (2002) "Tracer diffusion in granular shear flows", *Phys. Rev. E* **66**, 021308.