

Tracer diffusion in granular shear flows

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Tracer diffusion in a granular gas in simple shear flow is analyzed. The analysis is made from a perturbation solution of the Boltzmann kinetic equation through first order in the gradient of the mole fraction of tracer particles. The reference state (zeroth-order approximation) corresponds to a Sonine solution of the Boltzmann equation, which holds for arbitrary values of the restitution coefficients. Due to the anisotropy induced in the system by the shear flow, the mass flux defines a diffusion tensor D_{ij} instead of a scalar diffusion coefficient. The elements of this tensor are given in terms of the restitution coefficients and mass and size ratios. The dependence of the diffusion tensor on the parameters of the problem is illustrated in the three-dimensional case. The results show that the influence of dissipation on the elements D_{ij} is in general quite important, even for moderate values of the restitution coefficients. In the case of self-diffusion (mechanically equivalent particles), the trends observed in recent molecular-dynamics simulations are similar to those obtained here from the Boltzmann kinetic theory.

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I. INTRODUCTION

Granular systems under rapid flow conditions can be modeled as a fluid of inelastic hard spheres. In the simplest model, the grains are taken to be smooth so that the inelasticity is characterized through a constant coefficient of normal restitution. The essential difference with respect to molecular fluids is the absence of energy conservation yielding modifications of the usual hydrodynamic equations. Due to the kinetic-energy dissipation in collisions, energy must be externally injected to the granular gas in order to achieve a stationary state. In some experimental situations, the granular system is driven into flow by the presence of a shear field. In this case, a steady state is possible when the amount of energy supplied by shearing work is balanced by that lost due to the inelastic cooling. The study of the rheological properties of this steady shear flow state has received a great deal of attention in recent years, especially in the case of one-component systems [1]. However, much less is known in the more complicated case of multicomponent mixtures of grains.

An interesting problem is the analysis of diffusion in granular shear flows. The understanding of mass transport in granular systems is of practical interest since, for instance, powders must frequently be mixed together before any sort of processing can begin. The self-diffusion phenomenon in granular flows was studied earlier. Experimental studies include both systems with macroscopic flows [2,3] and vertically vibrated systems [4]. Complementary computer simulation studies have also been carried out [5], with special emphasis on the influence of the solid volume fraction on the diffusive motion of the grains. In general, all these previous studies were limited to observing the diffusion in only one direction, usually the direction parallel to the velocity gradient. However, due to the anisotropy induced in the system by the presence of shear flow, a diffusion tensor is required to describe the diffusion process instead of a single diffusion coefficient. To the best of my knowledge, the only attempt to measure the elements of this self-diffusion tensor has been

made by Campbell [6]. He measured these elements via molecular-dynamics simulations by using both particle tracking and through velocity correlations. Both methods were found to agree with reasonable accuracy. Very recently [7], the self-diffusion coefficients have been experimentally measured in a granular system under Couette flow by employing image technology.

In the context of kinetic theory, studies on granular flows in mixtures are scarcer. Most of them [8] are based on a Navier-Stokes description and, therefore, they are restricted to small velocity gradients, which for the steady simple shear flow is equivalent to the low-dissipation limit. For this reason, the diffusion is only characterized by a single coefficient which is not affected by the presence of the shear field. In addition, although these studies permit in principle different temperatures for the two species, they assume equal partial granular temperatures T_i in the quasielastic limit. Nevertheless, given the intrinsic connection between the shear rate and dissipation in this problem, energy nonequpartition is expected as the restitution coefficient decreases. As a matter of fact, some recent results obtained in molecular-dynamics simulations of granular sheared mixtures [9] as well as in real experiments of vibrated mixtures in three [10] and two dimensions [11] clearly show the breakdown of energy equipartition. This implies that the temperatures T_i are different from the mixture temperature T . The consequences of this effect on the transport properties are in general significant, as has been recently found in the freely cooling case [12,13]. In conclusion, a consistent theory describing diffusion in granular shear flows must take into account both the tensorial character of the mass transport as well as the possibility of temperature differences.

The aim of this paper is to get the diffusion tensor in a binary granular mixture under simple shear flow in the framework of the Boltzmann equation. Due to the complexity of the general problem, here we consider the special case in which one of the components (say, for instance, the species 1) is present in tracer concentration. The tracer problem is more amenable to analytical treatment. First, the tracer

particles are directly enslaved to the granular gas, and second there are fewer parameters [14–16]. Therefore, in this situation one can assume that the velocity distribution function f_2 of the excess component (granular gas) obeys a (closed) nonlinear Boltzmann equation while the velocity distribution function f_1 of the tracer particles (impurities) satisfies a Boltzmann-Lorentz equation. The starting point of our study is a recent solution of the set of Boltzmann equations for a binary mixture of inelastic hard spheres under shear flow [17]. The corresponding Boltzmann-Lorentz equation for the impurities is solved by means of a perturbative scheme in powers of the gradient of the mole fraction of tracer particles. The main feature of this expansion is that the reference state around which we perturb is not restricted to small values of the shear rate, which for the steady shear flow problem is equivalent to an arbitrary degree of dissipation. In the first order of the expansion, the tracer diffusion tensor is identified from the mass flux. Explicit expressions for the nonzero elements of this tensor are obtained by using a first Sonine polynomial approximation. These elements are given in terms of the restitution coefficients and the parameters of the mixture (masses and sizes).

The plan of the paper is as follows. In Sec. II, we introduce the set of coupled Boltzmann equations describing the mixture and state the problem we are interested in. The state of the mixture in the absence of diffusion is analyzed and, in particular, the nonzero elements of the pressure tensor \mathbf{P}_2 of the granular gas are obtained in the leading Sonine approximation. Comparison of these results with previous theories is also presented. The section ends studying the state of tracer particles with special emphasis on the evaluation of the specific dependence of the temperature ratio T_1/T_2 on restitution coefficients, mass ratio, and size ratio. Section III deals with the perturbation scheme used to solve the Boltzmann-Lorentz equation of the tracer particles when the diffusion takes place in the system. This section contains the main results of the paper since we determine the tracer diffusion tensor in the first order of the expansion of the concentration gradient. The dependence of the nonzero elements of this tensor on the different parameters of the problem is illustrated in the three-dimensional case, showing a good qualitative agreement with Campbell's simulations [6]. Finally, in Sec. IV we close the paper with some concluding remarks.

II. DESCRIPTION OF THE PROBLEM: GRANULAR MIXTURE IN SIMPLE SHEAR FLOW

We consider a granular binary mixture composed by smooth inelastic disks ($d=2$) or spheres ($d=3$) of masses m_1 and m_2 and diameters σ_1 and σ_2 . Collisions between particles are inelastic and characterized by three constant restitution coefficients α_{11} , α_{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 . In the low-density regime, the one-particle velocity distribution functions $f_i(\mathbf{r}, \mathbf{v}_i; t)$ ($i=1,2$) obey the set of nonlinear Boltzmann kinetic equations,

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_1 \cdot \nabla\right) f_i(\mathbf{r}, \mathbf{v}_1; t) = \sum_j J_{ij}[\mathbf{v}_1 | f_i(t), f_j(t)], \quad (1)$$

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

$$J_{ij}[\mathbf{v}_1 | f_i, f_j] = \sigma_{ij}^{d-1} \int d\mathbf{v}_2 \int d\hat{\boldsymbol{\sigma}} \Theta(\hat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12}) (\hat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12}) \times [\alpha_{ij}^{-2} f_i(\mathbf{r}, \mathbf{v}'_1, t) f_j(\mathbf{r}, \mathbf{v}'_2, t) - f_i(\mathbf{r}, \mathbf{v}_1, t) f_j(\mathbf{r}, \mathbf{v}_2, t)]. \quad (2)$$

Here, d is the dimensionality of the system, $\sigma_{ij} = (\sigma_i + \sigma_j)/2$, $\hat{\boldsymbol{\sigma}}$ is a unit vector along their line of centers, Θ is the Heaviside step function, and $\mathbf{g}_{12} = \mathbf{v}_1 - \mathbf{v}_2$. 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,

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

where $\mu_{ij} = m_i/(m_i + m_j)$. At a hydrodynamic level, the relevant quantities are the number densities n_i , the flow velocity \mathbf{u} , and the “granular” temperature T . They are defined in terms of moments of the distribution f_i as

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

$$nT = \sum_i n_i T_i = \sum_i \int d\mathbf{v} \frac{m_i}{d} V^2 f_i(\mathbf{v}), \quad (5)$$

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

The collision operators conserve the particle number of each species and the total momentum, but the total energy is not conserved. This implies that

$$\sum_{i,j} \int d\mathbf{v} \frac{1}{2} m_i V^2 J_{ij}[\mathbf{v} | f_i, f_j] = -\frac{d}{2} n T \zeta, \quad (6)$$

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

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

The total cooling rate ζ can be expressed in terms of ζ_i as

$$\zeta = T^{-1} \sum_i x_i T_i \zeta_i, \quad (8)$$

where $x_i = n_i/n$ is the mole fraction of species i .

Let us now describe the problem we are interested in. We consider a granular binary mixture in which the masses and sizes of both species are arbitrary. Our aim is to analyze a diffusion problem in a mixture of grains driven into flow by the action of shear forces. Here, we consider the simple case of the tracer limit, namely a binary mixture in which one of the components (say, for instance, 1) is present in tracer concentration ($x_1 \ll 1$). In the tracer limit, one expects that the state of the granular gas is not affected by the presence of the tracer particles so that its velocity distribution function f_2 obeys a (closed) nonlinear Boltzmann equation. Furthermore, the mole fraction of tracer particles is so small that their mutual interactions can be neglected in the kinetic equation of f_1 . As a consequence, the velocity distribution function of tracer particles f_1 satisfies a (linear) Boltzmann-Lorentz equation. Let us start by describing the state of the mixture in the absence of diffusion.

A. Granular gas (excess component)

We assume that the granular gas is subjected to the simple shear flow. From a macroscopic point of view, this state is characterized by a constant linear velocity profile $\mathbf{u} = \mathbf{u}_2 = \mathbf{a} \cdot \mathbf{r}$, where the elements of the tensor \mathbf{a} are $a_{k\ell} = a \delta_{kx} \delta_{\ell y}$, a being the constant shear rate. In addition, the partial density $n \approx n_2$ and the granular temperature $T \approx T_2$ are uniform. The temporal variation of the granular temperature T_2 can be obtained from the Boltzmann equation (1) as

$$\frac{\partial p_2}{\partial t} = -a P_{2,xy} - \frac{d}{2} \zeta_2 p_2, \quad (9)$$

where $p_2 = n_2 T_2$,

$$\mathbf{P}_2 = m_2 \int d\mathbf{v} \mathbf{V} \mathbf{V} f_2 \quad (10)$$

is the pressure tensor of the gas, and in the tracer limit

$$\zeta_2 = -\frac{1}{dn_2 T_2} \int d\mathbf{v} m_2 V^2 J_{22}[\mathbf{v}|f_2, f_2]. \quad (11)$$

The balance of energy (9) shows the different nature of this state for molecular and granular systems. While for elastic fluids ($\zeta_2 = 0$) the temperature increases monotonically in time due to the viscous heating term $a P_{2,xy}$, a steady state is possible for granular systems when the viscous heating is exactly compensated by the collisional cooling term $(d/2) p_2 \zeta_2$. In that case, the shear stress $P_{2,xy}$ and the cooling rate ζ_2 are related by

$$a P_{2,xy} = -\frac{d}{2} \zeta_2 p_2. \quad (12)$$

As a consequence, for a given shear rate a , the (steady) temperature T_2 is a function of the restitution coefficient α_{22} . This steady state is what we want to analyze.

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} : $f_2(\mathbf{r}, \mathbf{v}) \rightarrow f_2(\mathbf{V})$. Consequently, the stationary Boltzmann equation for the excess component becomes

$$-a V_y \frac{\partial}{\partial V_x} f_2(\mathbf{V}) = J_{22}[\mathbf{V}|f_2, f_2]. \quad (13)$$

We are mainly interested in computing the nonzero elements of the pressure tensor \mathbf{P}_2 . These elements can be obtained by multiplying the Boltzmann equation (13) by $m_2 V_k V_\ell$ and integrating over \mathbf{V} . The result is

$$a_{km} P_{2,\ell m} + a_{\ell m} P_{2,km} = A_{k\ell}, \quad (14)$$

where

$$A_{k\ell} = m_2 \int d\mathbf{V} V_k V_\ell J_{22}[\mathbf{V}|f_2, f_2]. \quad (15)$$

To get an explicit expression for \mathbf{P}_2 one needs to compute the right-hand side of the set of Eq. (14). This requires the explicit knowledge of f_2 , which is not known even in the elastic limit. However, one expects to get a good estimate of the low moments of the Boltzmann collisional operator by expanding f_2 in Sonine polynomials and then to truncate the series after the first few terms. This approach is similar to the usual moment method for solving the Boltzmann equation in the elastic case. Therefore, we take the leading Sonine approximation,

$$f_2(\mathbf{V}) \rightarrow f_{2,M}(\mathbf{V}) \left[1 + \frac{m_2}{2T_2} \left(\frac{P_{2,k\ell}}{p_2} - \delta_{k\ell} \right) \times \left(V_k V_\ell - \frac{1}{d} V^2 \delta_{k\ell} \right) \right], \quad (16)$$

where $f_{2,M}$ is a Maxwellian distribution at the temperature of the gas, i.e.,

$$f_{2,M}(\mathbf{V}) = n_2 \left(\frac{m_2}{2\pi T_2} \right)^{d/2} \exp\left(-\frac{m_2 V^2}{2T_2} \right). \quad (17)$$

With the approximation (16), the integrals appearing in the expressions of the cooling rate ζ_2 and the collisional moment $A_{k\ell}$ can be explicitly evaluated. The details of the calculation are given in the Appendix. This allows us to get the explicit expressions of the nonzero elements of \mathbf{P}_2 . They are given by

$$P_{2,yy}^* = P_{2,zz}^* = \dots = P_{2,dd}^* = \frac{d+1+(d-1)\alpha_{22}}{2d+3-3\alpha_{22}}, \quad (18)$$

$$P_{2,xy}^* = -4d \frac{d+1+(d-1)\alpha_{22}}{(1+\alpha_{22})(2d+3-3\alpha_{22})^2} a^*, \quad (19)$$

$$P_{2,xx}^* = d - (d-1) P_{2,yy}^*, \quad (20)$$

$$a^{*2} = \frac{d+2}{32d} \frac{(1+\alpha_{22})(2d+3-3\alpha_{22})^2 (1-\alpha_{22}^2)}{d+1+(d-1)\alpha_{22}}. \quad (21)$$

Moreover, the (reduced) cooling rate ζ_2^* is

$$\zeta_2^* = \frac{d+2}{4d} (1 - \alpha_{22}^2). \quad (22)$$

Here, $P_2^* = P_2/p_2$, $a^* = a/\nu$, $\zeta_2^* = \zeta_2/\nu$, and ν is a characteristic collision frequency given by $\nu = p_2/\eta$, where η is the shear viscosity coefficient of the gas in the elastic limit, i.e.,

$$\eta = \frac{d+2}{8} \pi^{-(d-1)/2} \Gamma(d/2) \sigma_2^{-(d-1)} (m_2 T_2)^{1/2}. \quad (23)$$

Equations (18)–(22) generalize previous results derived in the three-dimensional case [17]. The expression (21) clearly indicates the intrinsic connection between the velocity gradient and dissipation in the system. As a matter of fact, given that $\alpha_{22} \leq 1$, the range of (reduced) shear rates is defined in the interval $0 \leq a^{*2} \leq (d+2)(3+2d)^2/32d(d+1)$. The parameter a^* can be considered as the relevant nonequilibrium parameter of the system. In the elastic limit ($\alpha_{22} = 1$, which implies $a^* = 0$), the equilibrium results of the molecular gas are recovered, i.e., $P_{2,k\ell}^* = \delta_{k\ell}$. As was said in the Introduction, the steady simple shear flow for a monocomponent granular fluid has been the subject of many previous works. Two interesting studies have been carried out by Jenkins and Richman for smooth inelastic disks [18] and by Brey *et al.* [19] for a d -dimensional system. The latter description has been subsequently extended to dense gases [20]. The approximated theory of Jenkins and Richman [18] is based on a generalized Maxwellian distribution to model the steady shear flow. On the other hand, Brey *et al.* [19] solved a kinetic model equation of the Boltzmann equation and compared their predictions for the reduced temperature, shear stress, and normal stress differences with Monte Carlo simulations. Comparison between kinetic model results and simulation shows in general a good agreement. Our results differ from those reported in Refs. [18] and [19], although for practical purposes, the discrepancies between the different approaches are quite small, even for moderate values of α_{22} . As an illustration, in Fig. 1 we compare the different theories for the (reduced) elements of the pressure tensor P_2^* in a two-dimensional system ($d=2$). It is seen that the agreement is remarkable, although the discrepancies slightly increase as the restitution coefficient decreases.

B. Tracer component

In the absence of diffusion, the velocity distribution function f_1 of tracer particles satisfies the steady kinetic equation

$$-a V_y \frac{\partial}{\partial V_x} f_1 = J_{12}[\mathbf{V}|f_1, f_2]. \quad (24)$$

The most relevant moment at this level of approximation is the pressure tensor P_1 defined as

$$P_1 = m_1 \int d\mathbf{V} \mathbf{V} \mathbf{V} f_1(\mathbf{V}). \quad (25)$$

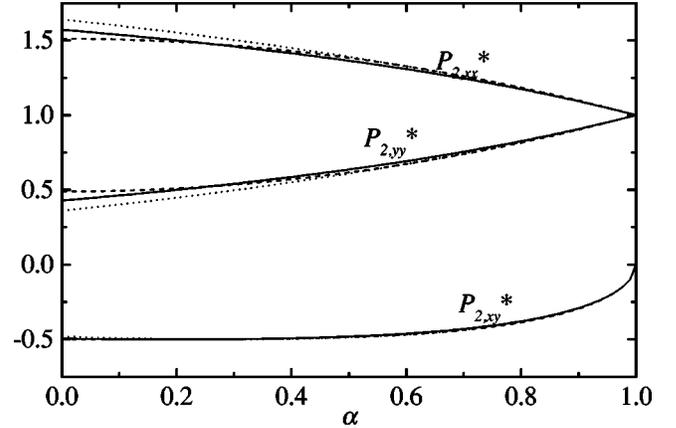


FIG. 1. Plot of the reduced elements of the pressure tensor of the granular gas as functions of the restitution coefficient $\alpha_{22} \equiv \alpha$ in the two-dimensional case. The solid lines correspond to the present theory, the dotted ones to that of Ref. [18], and the dashed ones to that of Ref. [19].

The nonzero elements of P_1 obey the set of equations

$$a_{km} P_{1,\ell m} + a_{\ell m} P_{1,km} = B_{k\ell}, \quad (26)$$

where

$$B_{k\ell} = m_1 \int d\mathbf{V} V_k V_\ell J_{12}[\mathbf{V}|f_1, f_2]. \quad (27)$$

As done before in the case of P_2 , we estimate the collisional moment $B_{k\ell}$ by taking the leading Sonine approximation of f_1 ,

$$f_1(\mathbf{V}) \rightarrow f_{1,M}(\mathbf{V}) \left[1 + \frac{m_1}{2T_1} \left(\frac{P_{1,k\ell}}{p_1} - \delta_{k\ell} \right) \times \left(V_k V_\ell - \frac{1}{d} V^2 \delta_{k\ell} \right) \right], \quad (28)$$

where $p_1 = n_1 T_1$ and now $f_{1,M}$ is a Maxwellian distribution at the temperature of the tracer particles T_1 , i.e.,

$$f_{1,M}(\mathbf{V}) = n_1 \left(\frac{m_1}{2\pi T_1} \right)^{d/2} \exp\left(-\frac{m_1 V^2}{2T_1} \right). \quad (29)$$

As will be shown later, the partial temperatures T_1 and T_2 are in general different so that the granular energy per particle is not equally distributed between both species.

Once the collisional moment $B_{k\ell}$ is determined (see the Appendix), the (reduced) nonzero components of $P_1^* = P_1/x_1 p_2$ can be easily obtained from Eq. (26). These components can be written in terms of the temperature ratio $\gamma = T_1/T_2$, the restitution coefficients α_{22} and α_{12} , and the parameters of the mixture. After some algebra, one gets

$$P_{1,yy}^* = P_{1,zz}^* = \dots = P_{1,dd}^* = -\frac{F + H P_{2,yy}^*}{G}, \quad (30)$$

$$P_{1,xy}^* = \frac{a^* P_{1,yy}^* - H P_{2,xy}^*}{G}, \quad (31)$$

$$P_{1,xx}^* = d\gamma - (d-1)P_{1,yy}^*, \quad (32)$$

where

$$F = \frac{\sqrt{2}}{2d} \left(\frac{\sigma_{12}}{\sigma_{22}} \right)^{d-1} \mu_{12} \left(\frac{1+\theta}{\theta^3} \right)^{1/2} (1+\alpha_{12}) \times \left[1 + \frac{\mu_{21}}{2} (d-1)(1+\theta)(1+\alpha_{12}) \right], \quad (33)$$

$$G = -\frac{\sqrt{2}}{4d} \left(\frac{\sigma_{12}}{\sigma_{22}} \right)^{d-1} \mu_{21} \left(\frac{1}{\theta(1+\theta)} \right)^{1/2} (1+\alpha_{12}) \times \{ 2[(d+2)\theta + d + 3] - 3\mu_{21}(1+\theta)(1+\alpha_{12}) \}, \quad (34)$$

$$H = \frac{\sqrt{2}}{4d} \left(\frac{\sigma_{12}}{\sigma_{22}} \right)^{d-1} \mu_{12} \left(\frac{1}{\theta(1+\theta)} \right)^{1/2} (1+\alpha_{12}) \times [3\mu_{21}(1+\theta)(1+\alpha_{12}) - 2]. \quad (35)$$

Here, $\theta = m_1 T_2 / m_2 T_1$ is the mean-square velocity of the gas particles relative to that of the tracer particles. To close the problem at this stage of approximation, it still remains to get the temperature ratio γ . It can be obtained, for instance, from the requirements (12) and its corresponding counterpart for species 1. This yields

$$\gamma = \frac{\zeta_2^* P_{1,xy}^*}{\zeta_1^* P_{2,xy}^*}, \quad (36)$$

where the cooling rate $\zeta_1^* = \zeta_1 / \nu$ for the tracer particles is (see the Appendix)

$$\zeta_1^* = \frac{(d+2)\sqrt{2}}{4d} \left(\frac{\sigma_{12}}{\sigma_2} \right)^{d-1} \mu_{21} \left(\frac{1+\theta}{\theta} \right)^{1/2} (1+\alpha_{12}) \times [2 - \mu_{21}(1+\theta)(1+\alpha_{12})]. \quad (37)$$

The solution to Eq. (36) gives γ as a function of the restitution coefficients α_{22} and α_{12} and the mechanical parameters of the mixture, i.e., the mass ratio $\mu = m_1 / m_2$ and the size ratio $w = \sigma_1 / \sigma_2$. Except for some limiting cases, Eq. (36) must be solved numerically. Thus, in the elastic case ($\alpha_{22} = \alpha_{12} = 1$), we recover the well-known equilibrium results with $\gamma = 1$ and $\theta \rightarrow m_1 / m_2$ as required by the equipartition theorem. In the case of mechanically equivalent particles ($m_1 = m_2$, $\alpha_{22} = \alpha_{12}$, $\sigma_1 = \sigma_2$), Eqs. (18)–(22) and (30)–(35) lead to $P_2^* = P_1^*$ and $\zeta_2^* = \zeta_1^*$, so that $\gamma = 1$. Beyond the above limit cases, as expected, our results yield $\gamma \neq 1$. The violation of energy equipartition in driven granular mixtures has been recently observed in molecular-dynamics simulations of sheared mixtures [9] and in real experiments [10,11]. This effect is generic of multicomponent granular systems and is consistent with previous results derived in the

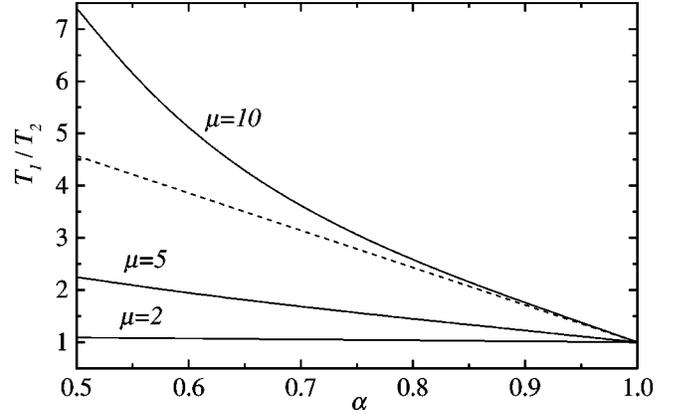


FIG. 2. Dependence of the temperature ratio $\gamma \equiv T_1/T_2$ on the restitution coefficient $\alpha_{22} = \alpha_{12} \equiv \alpha$ in the two-dimensional case for $w=2$ and three different values of the mass ratio μ . The dashed line corresponds to the prediction given by the theory of Jenkins and Mancini [21] in the case $\mu=5$.

unforced case [12,14–16]. To the best of my knowledge, the only previous theories including temperature differences have been proposed by Jenkins and Mancini [21] and by Huilin *et al.* [22]. However, both works are phenomenological with no attempt to solve the kinetic equation. Instead, they assume that the velocity distribution function is a local Maxwellian. This is reasonable for estimating the dense gas collisional transfer contributions to the fluxes, but not for evaluating their kinetic contributions. Both theories are applicable to a general flow field. In particular, the results obtained by Jenkins and Mancini [21] for the temperature ratio in the low-density limit for inelastic disks can be written as

$$\gamma = 1 - \frac{1+\mu}{1+w} \left[\frac{1+w}{2\mu} (1-\alpha_{12}) - \sqrt{\frac{\mu(1+\mu)}{2}} (1-\alpha_{22}) \right]. \quad (38)$$

In Fig. 2, we plot the temperature ratio γ versus the restitution coefficient α for a size ratio $w=2$ and three values of the mass ratio μ in the two-dimensional case ($d=2$). For the sake of simplicity, henceforth we will assume that the spheres or disks are made of the same material, i.e., $\alpha \equiv \alpha_{22} = \alpha_{12}$. Also for comparison, we show the prediction given by Eq. (38) in the case $\mu=5$. Important discrepancies between both theories appear even for values of α close to 1. As a matter of fact, the theory of Jenkins and Mancini predicts a violation of energy equipartition much more significant than our theory. It must be remarked that the quantitative predictions of our theory at the level of the temperature ratio have been recently confirmed by Monte Carlo simulations [17,23]. Regarding the influence of the parameters of the mixture, we observe that for large mass ratios the temperature differences are quite significant, even for moderate dissipation (say $\alpha \approx 0.9$). The temperature of the tracer particles is larger than that of the excess species when the tracer grains are heavier than the grains of the gas. This behavior has been also found in the recent computer simulations carried out in rapid shear flow [9].

III. TRACER DIFFUSION UNDER SIMPLE SHEAR FLOW

We want to study the diffusion of tracer particles immersed in a bath (granular gas) subjected to the simple shear flow. The diffusion process is induced in the system by a *weak* concentration gradient ∇x_1 . However, given that the strength of the shear rate a is arbitrary, the mass flux (which is generated by the gradient ∇x_1) can be modified by the presence of the shear flow. As stated above, in the tracer limit the state of particles of species 1 is mainly governed by the collisions with particles of species 2, so that the self-collisions among particles 1 can be neglected. Thus, the kinetic equation governing the evolution of the velocity distribution function f_1 reads

$$\frac{\partial}{\partial t} f_1 - a V_y \frac{\partial}{\partial V_x} f_1 + (V_k + a_{k\ell} r_\ell) \frac{\partial}{\partial r_k} f_1 = J_{12}[\mathbf{V}|f_1, f_2], \quad (39)$$

where here the derivative $\partial/\partial r_k$ is taken at constant \mathbf{V} . Tracer particles may freely exchange momentum and energy with the particles of the granular gas, and, therefore, these are not invariants of the collision operator $J_{12}[f_1, f_2]$. Only the number density of tracer particles is conserved. More specifically, the mole fraction x_1 obeys the conservation law

$$\left(\frac{\partial}{\partial t} + a_{k\ell} r_\ell \frac{\partial}{\partial r_k} \right) x_1 + \frac{\nabla \cdot \mathbf{j}_1}{m_1 n_2} = 0, \quad (40)$$

where the mass flux \mathbf{j}_1 is defined as

$$\mathbf{j}_1 = m_1 \int d\mathbf{V} \mathbf{V} f_1(\mathbf{V}). \quad (41)$$

When $\alpha_{22} = \alpha_{12} = 1$ (which gives $a^* = 0$), the well-known Fick law establishes a linear relationship between the mass flux \mathbf{j}_1 and the concentration gradient ∇x_1 . This law defines the diffusion coefficient. For finite values of the (reduced) shear rate a/ν (which means $\alpha_{22} \neq 1$), one expects that a generalized Fick's law holds but now a diffusion tensor rather than a scalar should appear. Our aim is to get this tensor in terms of α_{22} , α_{12} , μ , and w . To this end, and assuming that the mole fraction x_1 is slightly *nonuniform*, we solve Eq. (39) by means of a perturbation expansion around a nonequilibrium state with arbitrary shear rate, which is equivalent to strong dissipation in the simple shear flow [see Eq. (21)]. Thus, we write

$$f_1 = f_1^{(0)} + f_1^{(1)} + \dots, \quad (42)$$

where $f_1^{(k)}$ is of order k in ∇x_1 but applies for an *arbitrary* degree of dissipation since this distribution retains all the orders in a . The solution (42) qualifies as a normal solution since all the space and time dependence of f_1 occurs entirely through $x_1(\mathbf{r}; t)$ and their gradients. The zeroth-order approximation $f_1^{(0)}$ corresponds to the simple shear flow distribution but taking into account now the local dependence on the mole fraction x_1 . Although the explicit form of $f_1^{(0)}$ is not exactly known, only the knowledge of its second-degree mo-

ments (related to the pressure tensor \mathbf{P}_1) is necessary to get the diffusion tensor in the Sonine approximation.

The kinetic equation for $f_1^{(1)}$ can be obtained from the Boltzmann-Lorentz equation (39) by collecting all the terms of first order in ∇x_1 :

$$\begin{aligned} \frac{\partial}{\partial t} f_1^{(0)} - a V_y \frac{\partial}{\partial V_x} f_1^{(1)} + (V_k + a_{k\ell} r_\ell) \frac{\partial}{\partial r_k} f_1^{(0)} \\ = J_{12}[\mathbf{V}|f_1^{(1)}, f_2]. \end{aligned} \quad (43)$$

According to the balance equation (40), one has

$$\frac{\partial f_1^{(0)}}{\partial t} = \frac{\partial f_1^{(0)}}{\partial x_1} \frac{\partial x_1}{\partial t} = -a_{k\ell} r_\ell \frac{\partial x_1}{\partial r_k} \frac{\partial f_1^{(0)}}{\partial x_1}, \quad (44)$$

where use has been made of the fact that the zeroth-order approximation to the mass flux vanishes, i.e., $\mathbf{j}_1^{(0)} = \mathbf{0}$. Moreover,

$$\frac{\partial f_1^{(0)}}{\partial r_k} = \frac{\partial f_1^{(0)}}{\partial x_1} \frac{\partial x_1}{\partial r_k}. \quad (45)$$

Using Eqs. (44) and (45), Eq. (43) can be written as

$$\left(a V_y \frac{\partial}{\partial V_x} + \Lambda \right) f_1^{(1)} = \frac{\partial f_1^{(0)}}{\partial x_1} (\mathbf{V} \cdot \nabla x_1), \quad (46)$$

where Λ is the Boltzmann-Lorentz collision operator

$$\Lambda f_1^{(1)} = J_{12}[\mathbf{V}|f_1^{(1)}, f_2]. \quad (47)$$

The solution to Eq. (46) is proportional to ∇x_1 , i.e., it has the form

$$f_1^{(1)}(\mathbf{V}) = \mathcal{A}(\mathbf{V}) \cdot \nabla x_1. \quad (48)$$

Substitution of this into Eq. (46) yields

$$\left(a V_y \frac{\partial}{\partial V_x} + \Lambda \right) \mathcal{A} = \frac{\partial f_1^{(0)}}{\partial x_1} \mathbf{V}. \quad (49)$$

The first-order approximation to the mass flux is given by

$$\mathbf{j}_1^{(1)} = m_1 \int d\mathbf{V} \mathbf{V} f_1^{(1)}(\mathbf{V}) = -\mathbf{D} \cdot \nabla x_1, \quad (50)$$

where the tracer diffusion tensor is

$$D_{k\ell} = -m_1 \int d\mathbf{V} V_k \mathcal{A}_\ell(\mathbf{V}). \quad (51)$$

The solution to the integral equation (49) allows one to determine the quantity \mathcal{A} . From this solution one can determine the tracer diffusion tensor by means of Eq. (51).

In order to get an explicit expression for the tensor \mathbf{D} , we need to know the quantity \mathcal{A} . A good estimate of \mathcal{A} to evaluate the mass flux $\mathbf{j}_1^{(1)}$ is given by the first Sonine approximation, in which only the leading term in the expansion of $\mathcal{A}(\mathbf{V})$ in Sonine polynomials is kept. Thus, we take the following approximation to \mathcal{A} :

$$A(\mathbf{V}) \rightarrow -\frac{1}{n_1 T_1} \mathbf{V} \cdot \mathbf{D} f_{1,M}(\mathbf{V}). \quad (52)$$

Using Eq. (52), an equation for the diffusion tensor is easily derived from Eq. (49). The result can be written as

$$(\mathbf{a} + \mathbf{\Omega}) \cdot \mathbf{D} = p_2 \mathbf{P}_1^*, \quad (53)$$

where the nonzero components of \mathbf{P}_1^* are given by Eqs. (30)–(32) and we have introduced the tensorial quantity

$$\mathbf{\Omega} = -\frac{m_1}{n_1 T_1} \int d\mathbf{V} \mathbf{V} \mathbf{V} \wedge \mathbf{V} f_{1,M}. \quad (54)$$

The expression of the tensor $\mathbf{\Omega}$ has been obtained in the Appendix with the result

$$\begin{aligned} \mathbf{\Omega} = & \frac{2}{d} \frac{\pi^{(d-1)/2}}{\Gamma(d/2)} n_2 \mu_{21} \sigma_{12}^{d-1} (2T_2/m_2)^{1/2} (1 + \alpha_{12}) \\ & \times [(1 + \theta)\theta]^{-1/2} \left[\left(1 + \frac{d+1}{d+2} \theta \right) \mathbf{1} + \frac{\theta}{d+2} \mathbf{P}_2^* \right]. \quad (55) \end{aligned}$$

The solution of Eq. (53) is

$$\mathbf{D} = p_2 (\mathbf{a} + \mathbf{\Omega})^{-1} \cdot \mathbf{P}_1^*. \quad (56)$$

Equation (56) is the primary result of this paper. It provides an explicit expression of the tracer diffusion tensor of a granular binary mixture in simple shear flow. The elements of this tensor give all the information on the physical mechanisms involved in the diffusion of tracer particles in a strongly sheared granular gas. In the absence of shear rate (which is equivalent to $\alpha_{22} = \alpha_{12} = 1$), $D_{k\ell} = D_0 \delta_{k\ell}$, where

$$D_0 = \frac{d}{4\sqrt{2}} \frac{\Gamma(d/2)}{\pi^{(d-1)/2} \sigma_{12}^{d-1}} \sqrt{\mu(1+\mu)} (m_2 T_2)^{1/2} \quad (57)$$

is the tracer diffusion coefficient of a molecular gas [24]. As the restitution coefficients decrease, rheological effects become important and the elements of the diffusion tensor are different from the one obtained in the equilibrium case. The dependence of the diffusion coefficients on the restitution coefficients α_{22} and α_{12} as well as on the mass ratio μ and the size ratio w is highly nonlinear. As happens for elastic fluids [25], Eq. (56) shows that diffusion under simple shear flow is a very complex problem due basically to the anisotropy induced in the system by the shear flow.

To illustrate the dependence of the elements $D_{k\ell}$ on the parameters of the problem, let us consider a mixture of inelastic hard spheres ($d=3$). According to Eq. (56), $D_{xz} = D_{zx} = D_{yz} = D_{zy} = 0$, in agreement with the symmetry of the problem. Consequently, there are five relevant elements: the three diagonal and two (D_{xy} , D_{yx}) off-diagonal elements. In general, $D_{xx} \neq D_{yy} \neq D_{zz}$ and $D_{xy} \neq D_{yx}$. The off-diagonal elements measure cross effects in the diffusion of particles induced by the shear flow. Thus, for instance, D_{xy} gives the transport of mass along the direction of the flow of

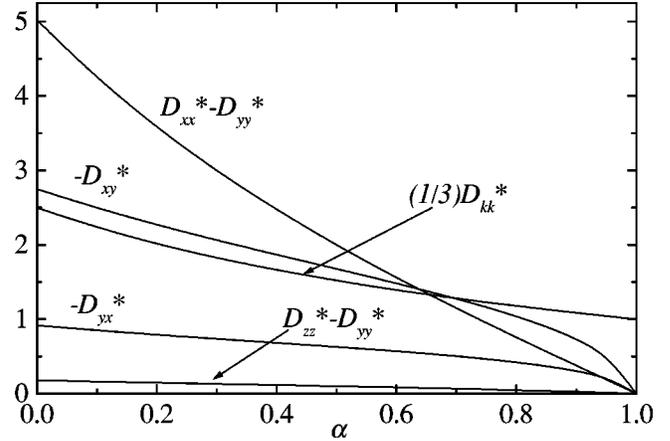


FIG. 3. Dependence of the diagonal and off-diagonal elements of the reduced self-diffusion tensor \mathbf{D}^* on the restitution coefficient $\alpha_{22} = \alpha_{12} \equiv \alpha$ in the three-dimensional case.

the system (x axis) due to a concentration gradient parallel to the gradient of the flow velocity (y axis). Both off-diagonal elements are negative.

Before analyzing the influence of the mechanical parameters of the mixture on diffusion, it is instructive to explore the particular case of self-diffusion, i.e., when the tracer particles are mechanically equivalent to the gas particles. This situation involves only single-particle motion and it is therefore somewhat simpler to compute the diffusion coefficients. In particular, the temperature of the tracer particles is the same as that of the gas particles and so $\theta = 1$ in Eqs. (30)–(35) and (55). In Fig. 3, we plot $D_{xx}^* - D_{yy}^*$, $D_{zz}^* - D_{yy}^*$, $(D_{xx}^* + D_{yy}^* + D_{zz}^*)/3 \equiv (1/3)D_{kk}^*$, $-D_{xy}^*$, and $-D_{yx}^*$ as functions of the restitution coefficient $\alpha \equiv \alpha_{12} = \alpha_{22}$. Here, $D_{ij}^* \equiv D_{ij}/D_0$, with D_0 given by Eq. (57). We see that the deviation from the functional form for elastic collisions is quite important even for moderate dissipation. Thus, for instance at $\alpha = 0.8$, $D_{xx}^* - D_{yy}^* \approx 0.76$, $D_{zz}^* - D_{yy}^* \approx 0.046$, $(1/3)D_{kk}^* \approx 1.18$, $-D_{xy}^* \approx 1.039$, and $-D_{yx}^* \approx 0.42$. The figure also shows that the anisotropy of the system, as measured by the differences $D_{xx}^* - D_{yy}^*$ and $D_{zz}^* - D_{yy}^*$, grows with the inelasticity. This anisotropy is much more important in the plane of shear flow ($D_{xx}^* - D_{yy}^*$) than in the plane perpendicular to the flow velocity ($D_{zz}^* - D_{yy}^*$). This is basically due to the fact that $P_{s,xx}^* \neq P_{s,yy}^* = P_{s,zz}^*$ with $s = 1, 2$.

As said before, Campbell [6] has carried out molecular-dynamics simulations to measure the nonzero elements of the self-diffusion tensor. In his work, the self-diffusion coefficients were nondimensionalized by the product of the shear rate and the particle diameter. In our units, this corresponds to the reduced tensor $\tilde{D}_{ij} = D_{ij}^*/a^*$. Although the solid fractions analyzed in his simulations prevent us in general from making a quantitative comparison between our theory (restricted to dilute gases) and his computer simulations, we observe that the general qualitative dependence of the self-diffusion tensor on dissipation agrees well with our results, at least for the lowest solid fraction considered. Thus, theory and simulation predict that the magnitude of the normal diffusion coefficients follow the pattern $\tilde{D}_{xx} > \tilde{D}_{zz} > \tilde{D}_{yy}$ while,

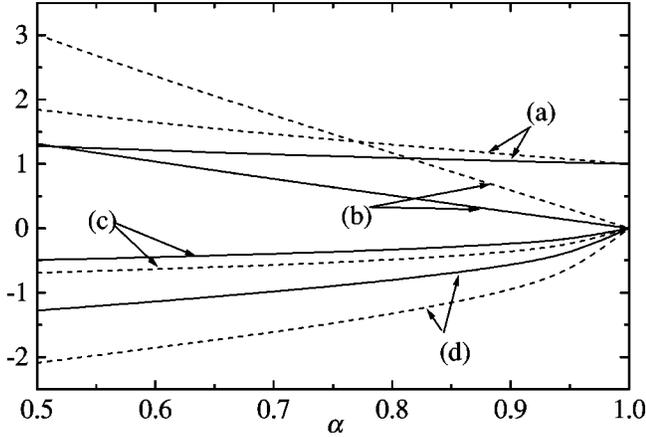


FIG. 4. Dependence of the scalar (a) $\frac{1}{3}D_{kk}^*$, the difference (b) $D_{xx}^* - D_{yy}^*$, and the off-diagonal elements (c) D_{xy}^* and (d) D_{yx}^* of the reduced tracer diffusion tensor D^* on the restitution coefficient $\alpha_{22} = \alpha_{12} \equiv \alpha$ in the three-dimensional case for $w=2$ and two values of the mass ratio μ : $\mu=2$ (solid lines) and $\mu=4$ (dashed lines).

in general, the elements \tilde{D}_{ij} decrease as the restitution coefficient decreases. An exception to the latter rule is the element \tilde{D}_{xx} , which does not depend sensitively on α . On the other hand, in Campbell's simulation work [6], he found that the values of $-\tilde{D}_{xy}$ were roughly of the same magnitude as \tilde{D}_{yy} provided that the solid fraction is smaller than 0.4. This trend is not completely followed by our theory since the values of $-\tilde{D}_{xy}$ and \tilde{D}_{yy} are significantly different for highly inelastic spheres. Thus, for instance, at $\alpha=0.8$, $-\tilde{D}_{xy} \approx 2.43$ and $\tilde{D}_{yy} \approx 2.15$ but $-\tilde{D}_{xy} \approx 2.54$ and $\tilde{D}_{yy} \approx 1.10$ at $\alpha=0.4$.

The dependence of the diffusion coefficients D_{ij}^* on the restitution coefficient for different values of the mass ratio μ is illustrated in Fig. 4. In this case, we take a size ratio $w=2$ and two values of the mass ratio: $\mu=2$ and $\mu=4$. For a given value of the inelasticity, we observe that the deviations from the elastic results are more important as the tracer particles are heavier than the gas particles.

IV. CONCLUDING REMARKS

In this paper, we have described diffusion of tracer particles in a granular gas subjected to the simple shear flow. We have been interested in the steady state where the effect of viscosity is compensated for by the dissipation in collisions. Under these conditions, the resulting diffusion is anisotropic and, thus, cannot be described by a single diffusion coefficient. Instead, it must be described by a diffusion tensor whose explicit determination has been the main objective of this work. In order to capture the essential aspects of such a nonlinear problem, we have considered here a granular mixture in the low-density regime as a prototype granular system, which lends itself to a detailed description by means of the nonlinear Boltzmann kinetic equation.

We have been concerned with the physical situation where a weak concentration gradient coexists with a strong shear rate, which for the steady simple shear flow problem

means strong dissipation. For this reason, the Boltzmann-Lorentz equation corresponding to the tracer particles has been solved by means of a perturbation expansion around a *nonequilibrium* sheared state. This implies that the different approximations of this expansion are *nonlinear* functions of the restitution coefficients as well as of the parameters of the mixture (mass and size ratios). To get explicit results, we have used a first Sonine polynomial approximation to evaluate the cooling rates and the collisional moments of the Boltzmann operators. The reliability of this approximation has been recently assessed in the (pure) shear flow problem where it has been shown to agree very well with Monte Carlo simulations in the case of hard spheres [17].

The kinetic theory results show that the elements D_{ij} of the diffusion tensor present a complex dependence on the restitution coefficients α_{22} and α_{12} and on the mass ratio $\mu = m_1/m_2$ and the size ratio $w = \sigma_1/\sigma_2$. In the elastic case, $\alpha_{ij}=1$, $D_{ij}=D_0\delta_{ij}$, where D_0 is given by Eq. (57) and one recovers the expression of the diffusion coefficient for normal fluids. The deviations of the tensor D_{ij} from the scalar D_0 have two distinct origins. First, the presence of shear flow gives rise to the new tensorial term $\mathbf{a} + \mathbf{\Omega}$ on the left-hand side of Eq. (53) instead of the corresponding collision frequency of the elastic diffusion problem. Second, given that the tracer and fluid particles are mechanically different, the reference state (zeroth-order approximation of the expansion) of tracer particles is completely different from that of the gas particles. In particular, when $\mu \neq 1$ and/or $w \neq 1$, the temperature ratio γ is clearly different from 1 (as can be seen in Fig. 2), confirming the breakdown of the energy equipartition. The effect of different temperatures for the tracer and gas particles is expressed by the appearance of $\theta = \mu/\gamma$ in \mathbf{P}_1 [cf. Eqs. (30)–(32)] and in $\mathbf{\Omega}$. Each one of the two aforementioned effects is a different reflection of dissipation present in the system.

A simple case is the self-diffusion problem, i.e., when the tracer and gas particles are mechanically equivalent. In this case, $\mathbf{P}_2^* = \mathbf{P}_1^*$ and $\gamma=1$. This situation has been previously studied by Campbell [6] by means of molecular-dynamics simulations. As has been discussed in Sec. III, our predictions for the self-diffusion tensor agree qualitatively well with these simulations. On the other hand, when the tracer and gas particles are mechanically *different*, to my knowledge no previous studies on the diffusion tensor under shear flow have been made. As pointed out in the Introduction, most of the works on granular mixtures [8] are based on the Chapman-Enskog expansion around a local equilibrium state up to the Navier-Stokes order, and therefore they are restricted to the low-dissipation limit in the simple shear flow. In addition, they also assume a single temperature to describe the mixture. A more careful calculation which takes into account temperature differences has been recently made by Garzó and Dufty [13,14]. They have obtained explicit expressions for the transport coefficients of a granular binary mixture in terms of the restitution coefficients and the parameters of the mixture. Since these results have been derived taking the freely cooling state as the reference one, the diffusion is characterized by a single scalar coefficient that cannot be directly compared to the diffusion tensor obtained

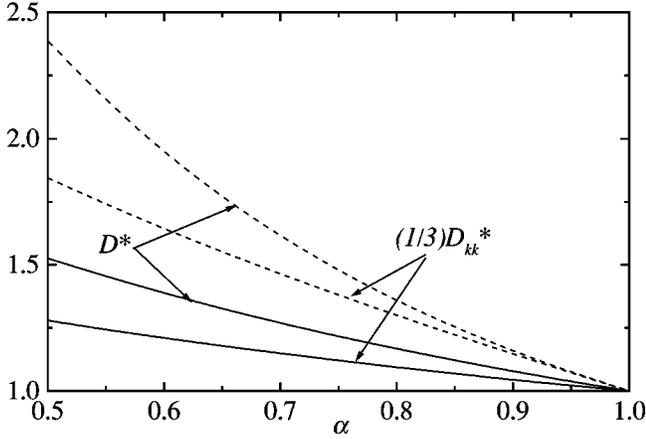


FIG. 5. Plot of the scalar $\frac{1}{3}D_{kk}^*$ and the reduced diffusion coefficient D^* obtained in Ref. [13] as functions of the restitution coefficient $\alpha_{22}=\alpha_{12}\equiv\alpha$ in the three-dimensional case for $w=2$ and two values of the mass ratio μ : $\mu=2$ (solid lines) and $\mu=4$ (dashed lines).

here. However, it would be interesting to compare the diffusion results obtained here in the driven sheared case with those found in the unforced case [13]. In Fig. 5, we have compared the behavior of the scalar $\frac{1}{3}D_{kk}^*$ (which can be understood as a generalized mutual diffusion coefficient in a sheared mixture) with the (reduced) diffusion coefficient D^* obtained in Ref. [13] in the tracer limit ($x_1\rightarrow 0$). We observe that, although the reference states in both descriptions are very different, the dependence of both diffusion coefficients on dissipation is quite similar since they increase as α increases. This trend is more significant in the unforced case than in the sheared case.

The evaluation of the diffusion tensor for practical purposes requires the truncation of a Sonine polynomial expansion. In the case of the (pure) simple shear flow problem, recent Monte Carlo simulations [17,23] have shown the accuracy of the leading-order truncation. We expect that this agreement may be extended to the elements of the diffusion tensor for a wide range of values of dissipation. Exceptions to this agreement could be disparate mass binary mixtures (e.g., electron-proton systems) for which the first Sonine solution is not perhaps a good approximation and higher-order terms should be considered. We hope that the results derived in this paper will stimulate the performance of computer simulations to check the quality of the approximations given here for the diffusion tensor. Given the difficulties associated with molecular-dynamics simulations in the low-density regime, one could perhaps use the direct simulation Monte Carlo method [26], which is being shown to be fruitful in the context of granular systems.

ACKNOWLEDGMENTS

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APPENDIX: EVALUATION OF ζ_i , A , B , AND Ω

In this appendix, we evaluate the cooling rates ζ_i , the collisional velocity moments A and B , and the tensorial collision frequency Ω by using the corresponding leading Sonine approximations.

1. Evaluation of ζ_i

The cooling rate ζ_1 of the tracer particles is defined as

$$\zeta_1 = -\frac{1}{dn_1 T_1} \int d\mathbf{V}_1 m_1 V_1^2 J_{12}[\mathbf{V}_1 | f_1, f_2]. \quad (\text{A1})$$

A useful identity for an arbitrary function $h(\mathbf{V}_1)$ is given by

$$\begin{aligned} & \int d\mathbf{V}_1 h(\mathbf{V}_1) J_{12}[\mathbf{V}_1 | f_1^{(0)}, f_2] \\ &= \sigma_{12}^{d-1} \int d\mathbf{V}_1 \int d\mathbf{V}_2 f_1^{(0)}(\mathbf{V}_1) f_2(\mathbf{V}_2) \\ & \quad \times \int d\hat{\boldsymbol{\sigma}} \Theta(\hat{\boldsymbol{\sigma}} \cdot \mathbf{g})(\hat{\boldsymbol{\sigma}} \cdot \mathbf{g}) [h(\mathbf{V}_1'') - h(\mathbf{V}_1)], \end{aligned} \quad (\text{A2})$$

with

$$\mathbf{V}_1'' = \mathbf{V}_1 - \mu_{21}(1 + \alpha_{12})(\hat{\boldsymbol{\sigma}} \cdot \mathbf{g})\hat{\boldsymbol{\sigma}}. \quad (\text{A3})$$

Using Eq. (A2), Eq. (A1) can be written as

$$\begin{aligned} \zeta_1 &= -\frac{m_1}{dn_1 T_1} \sigma_{12}^{d-1} (1 + \alpha_{12}) \mu_{21} \int d\mathbf{V}_1 \int d\mathbf{V}_2 f_1(\mathbf{V}_1) f_2(\mathbf{V}_2) \\ & \quad \times \int d\hat{\boldsymbol{\sigma}} \Theta(\hat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12})(\hat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12})^2 \\ & \quad \times [\mu_{21}(1 + \alpha_{12})(\hat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12}) - 2(\mathbf{V}_1 \cdot \hat{\boldsymbol{\sigma}})]. \end{aligned} \quad (\text{A4})$$

To perform the angular integrations, we need the results

$$\int d\hat{\boldsymbol{\sigma}} \Theta(\hat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12})(\hat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12})^n = \beta_n g_{12}^n, \quad (\text{A5})$$

$$\int d\hat{\boldsymbol{\sigma}} \Theta(\hat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12})(\hat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12})^n \hat{\boldsymbol{\sigma}} = \beta_{n+1} g_{12}^{n-1} \mathbf{g}_{12}, \quad (\text{A6})$$

where

$$\beta_n = \pi^{(d-1)/2} \frac{\Gamma((n+1)/2)}{\Gamma((n+d)/2)}. \quad (\text{A7})$$

Thus, the integration over $\hat{\boldsymbol{\sigma}}$ in Eq. (A4) leads to

$$\begin{aligned} \zeta_1 &= \frac{m_1}{dn_1 T_1} \sigma_{12}^{d-1} \beta_3 (1 + \alpha_{12}) \mu_{21} \int d\mathbf{V}_1 \int d\mathbf{V}_2 f_1(\mathbf{V}_1) f_2(\mathbf{V}_2) \\ & \quad \times [\mu_{21} g_{12}^3 (1 - \alpha_{12}) + 2g_{12}(\mathbf{g}_{12} \cdot \mathbf{G}_{12})], \end{aligned} \quad (\text{A8})$$

where $\mathbf{G}_{12} = \mu_{12}\mathbf{V}_1 + \mu_{21}\mathbf{V}_2$ is the center-of-mass velocity. Now, we take the Sonine approximations given by Eq. (16) for f_2 and Eq. (28) for f_1 . Neglecting nonlinear terms in the tensors $\mathbf{C}_i \equiv \mathbf{P}_i^* - \mathbb{1}$, one gets

$$\zeta_1 = \frac{m_1 n_2}{dT_1} \sigma_{12}^{d-1} v_0^3 \beta_3 \mu_{21} (1 + \alpha_{12}) \theta^{d/2} I_\zeta(\theta), \quad (\text{A9})$$

where

$$I_\zeta(\theta) = \pi^{-d} \int d\mathbf{V}_1^* \int d\mathbf{V}_2^* g_{12}^* [\mu_{21} g_{12}^{*2} (1 - \alpha_{12}) + 2(\mathbf{g}_{12}^* \cdot \mathbf{G}_{12}^*)] e^{-\theta v_1^{*2} - v_2^{*2}}. \quad (\text{A10})$$

Here, $\mathbf{V}_i^* = \mathbf{V}_i/v_0$, $\mathbf{g}_{12}^* = \mathbf{g}_{12}/v_0$, $\mathbf{G}_{12}^* = \mathbf{G}_{12}/v_0$, $\theta = \mu_{12}/(\mu_{21}\gamma)$, $\gamma = T_1/T_2$, and $v_0 = \sqrt{2T_2/m_2}$. In Eqs. (A9) and (A10), use has been made of the fact that the scalar ζ_1 cannot be coupled to the traceless tensor \mathbf{C}_i so that the only contributions to ζ_1 come from the (pure) Maxwellian terms in Eqs. (16) and (28). The integral I_ζ can be evaluated by the change of variables

$$\mathbf{x} = \mathbf{V}_1^* - \mathbf{V}_2^*, \quad \mathbf{y} = \theta \mathbf{V}_1^* + \mathbf{V}_2^*, \quad (\text{A11})$$

with the Jacobian $(1 + \theta)^{-d}$. The integral $I_\zeta(\theta)$ can be now easily computed with the result

$$I_\zeta(\theta) = \frac{\Gamma((d+3)/2)}{\Gamma(d/2)} \theta^{-(d+3)/2} (1 + \theta)^{1/2} \times [2 - \mu_{21}(1 + \theta)(1 + \alpha_{12})]. \quad (\text{A12})$$

Use of the result (A12) in Eq. (A9) yields

$$\zeta_1 = 2 \frac{\pi^{(d-1)/2}}{d\Gamma(d/2)} n_2 \sigma_{12}^{d-1} v_0 \mu_{21} (1 + \alpha_{12}) \left(\frac{1 + \theta}{\theta} \right)^{1/2} \times [2 - \mu_{21}(1 + \theta)(1 + \alpha_{12})]. \quad (\text{A13})$$

The corresponding expression for ζ_2 can be easily obtained from Eq. (A13) and the result is

$$\zeta_2 = \sqrt{2} \frac{\pi^{(d-1)/2}}{d\Gamma(d/2)} n_2 \sigma_2^{d-1} v_0 (1 - \alpha_{22}^2). \quad (\text{A14})$$

2. Evaluation of \mathbf{A} and \mathbf{B}

Since the tensor \mathbf{A} can be easily obtained from the expression of \mathbf{B} , let us explicitly evaluate the latter tensor. It is defined as

$$\mathbf{B} = \int d\mathbf{V}_1 m_1 \mathbf{V}_1 \mathbf{V}_1 J_{12}[\mathbf{V}_1 | f_1, f_2]. \quad (\text{A15})$$

Using Eq. (A2), Eq. (A15) can be written as

$$\begin{aligned} \mathbf{B} = & -m_1 \sigma_{12}^{d-1} \beta_3 \mu_{21} (1 + \alpha_{12}) \int d\mathbf{V}_1 \int d\mathbf{V}_2 f_1(\mathbf{V}_1) \\ & \times f_2(\mathbf{V}_2) g_{12} \left[\mathbf{g}_{12} \mathbf{G}_{12} + \mathbf{G}_{12} \mathbf{g}_{12} + \frac{\mu_{21}}{d+3} (2d+3-3\alpha_{12}) \right. \\ & \left. \times \mathbf{g}_{12} \mathbf{g}_{12} - \frac{\mu_{21}}{d+3} (1 + \alpha_{12}) g_{12}^2 \mathbb{1} \right], \end{aligned} \quad (\text{A16})$$

where use has been made of Eq. (A6) and

$$\int d\hat{\boldsymbol{\sigma}} \Theta(\hat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12}) (\hat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12})^n \hat{\boldsymbol{\sigma}} \hat{\boldsymbol{\sigma}} = \frac{\beta_n}{n+d} g_{12}^{n-2} (n \mathbf{g}_{12} \mathbf{g}_{12} + g_{12}^2 \mathbb{1}). \quad (\text{A17})$$

Substituting the Sonine approximations (16) and (28) for f_2 and f_1 , respectively, and retaining only linear terms in the tensors \mathbf{C}_i , one gets

$$\begin{aligned} \mathbf{B} = & -m_1 \sigma_{12}^{d-1} \beta_3 \mu_{21} (1 + \alpha_{12}) n_1 n_2 v_0^3 \theta^{d/2} \pi^{-d} \int d\mathbf{V}_1^* \int d\mathbf{V}_2^* g_{12}^* e^{-\theta v_1^{*2} - v_2^{*2}} \left[1 + \theta \mathbf{C}_1 : \left(\mathbf{V}_1^* \mathbf{V}_1^* - \frac{1}{d} v_1^{*2} \mathbb{1} \right) \right. \\ & \left. + \mathbf{C}_2 : \left(\mathbf{V}_2^* \mathbf{V}_2^* - \frac{1}{d} v_2^{*2} \mathbb{1} \right) \right] \left[\mathbf{g}_{12}^* \mathbf{G}_{12}^* + \mathbf{G}_{12}^* \mathbf{g}_{12}^* + \frac{\mu_{21}}{d+3} (2d+3-3\alpha_{12}) \mathbf{g}_{12}^* \mathbf{g}_{12}^* - \frac{\mu_{21}}{d+3} (1 + \alpha_{12}) g_{12}^{*2} \mathbb{1} \right]. \end{aligned} \quad (\text{A18})$$

This integral can be computed by the change of variables (A11). After a lengthy algebra, the result is

$$\begin{aligned} \mathbf{B} = & \frac{\pi^{(d-1)/2}}{d\Gamma(d/2)} \sigma_{12}^{d-1} m_1 n_1 n_2 \mu_{21} (1 + \alpha_{12}) v_0^3 \left(\frac{1 + \theta}{\theta} \right)^{3/2} \left\{ \left[\frac{\lambda_{12}}{d+2} + \frac{d}{d+3} \mu_{21} (1 + \alpha_{12}) \right] \mathbb{1} \right. \\ & \left. - 2 \frac{\theta}{(1 + \theta)^2} \left[\left(1 + \frac{(d+3)}{2(d+2)} \frac{1 + \theta}{\theta} \lambda_{12} \right) \gamma^{-1} \mathbf{P}_1^* - \left(1 - \frac{(d+3)}{2(d+2)} (1 + \theta) \lambda_{12} \right) \mathbf{P}_2^* \right] \right\}, \end{aligned} \quad (\text{A19})$$

where

$$\lambda_{12} = \frac{2}{1+\theta} - \frac{3}{d+3} \mu_{21}(1+\alpha_{12}). \quad (\text{A20})$$

The corresponding expression for A can be easily inferred from Eq. (A19) by just making the change $1 \rightarrow 2$ and $\theta \rightarrow 1$:

$$A = \frac{\sqrt{2} \pi^{(d-1)/2}}{2d(d+2)\Gamma(d/2)} \sigma_2^{d-1} m_2 n_2^2 v_0^3 (1+\alpha_{22}) \times \{[d+1+\alpha_{22}(d-1)] - (2d+3-3\alpha_{22})\mathbf{P}_2^*\}. \quad (\text{A21})$$

3. Evaluation of Ω

The tensor Ω is defined as

$$\Omega = -\frac{m_1}{n_1 T_1} \int d\mathbf{V}_1 \mathbf{V}_1 J_{12}[\mathbf{V}_1 f_{1,M}, f_2]. \quad (\text{A22})$$

The evaluation of Ω can be made following similar mathematical steps as above. Thus, using Eq. (A1) and the Sonine approximation to f_2 in Eq. (A22), one gets

$$\begin{aligned} \Omega &= \frac{m_1}{T_1} \pi^{-d} \sigma_{12}^{d-1} \mu_{21}(1+\alpha_{12}) \beta_3 n_2 v_0^3 \theta^{d/2} \int d\mathbf{V}_1^* \int d\mathbf{V}_2^* g_{12}^* g_{12}^* \mathbf{V}_1^* \left[1 + \mathbf{C}_2 : \left(\mathbf{V}_2^* \mathbf{V}_2^* - \frac{1}{d} V_2^{*2} \mathbf{1} \right) \right] e^{-\theta V_1^{*2} - V_2^{*2}} \\ &= 2n_2 \pi^{-d} \mu_{21}(1+\alpha_{12}) \sigma_{12}^{d-1} \theta^{d/2+1} v_0 \beta_3 (1+\theta)^{-(1+d)} \int d\mathbf{x} \int d\mathbf{y} \mathbf{x} \mathbf{x}(\mathbf{x}+\mathbf{y}) [1 + (1+\theta)^{-2} \mathbf{C}_2 : (\mathbf{y} - \theta \mathbf{x})(\mathbf{y} - \theta \mathbf{x})] \\ &\quad \times e^{-bx^2 - cy^2}, \end{aligned} \quad (\text{A23})$$

where $b = \theta(1+\theta)^{-1}$ and $c = (1+\theta)^{-1}$. This integral is easily performed, with the result

$$\Omega = \frac{2}{d} \frac{\pi^{(d-1)/2}}{\Gamma(d/2)} \mu_{21} \sigma_{12}^{d-1} n_2 v_0 (1+\alpha_{12}) \left(\frac{1+\theta}{\theta} \right)^{1/2} \left[1 + \frac{1}{d+2} \frac{\theta}{1+\theta} (\mathbf{P}_2^* - 1) \right]. \quad (\text{A24})$$

This expression yields Eq. (55) given in the text.

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