How good is the equipartition assumption for the transport properties of a granular mixture?

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Abstract Kinetic-theory, with the assumption of *equipartition* of granular energy, suggests that the pressure and viscosity of a granular mixture vary *monotonically* with the mass-ratio. Our simulation results show a *non-monotonic* behaviour that can be explained qualitatively by a simple model allowing for *non-equipartition* of granular energy between the species with different mass.

Keywords Binary mixture, event-driven simulation, energy non-equipartition, transport coefficients, mixture theory

1 Introduction

The balance laws and the constitutive relations for the transport properties of bidisperse granular mixtures have been proposed by Jenkins & Mancini [1,2], using the analogy with dense-gas kinetic theory of mixtures [3,4]. Some important modifications in these models were recently incorporated by Willits & Arnarson [5,6]. All the above mentioned models are first-order in inelasticity, meaning that they are valid for nearly elastic particles. A further important assumption is that the fluctuation kinetic energy is *equally* partitioned between the two species. Recent theoretical studies [7–10] show that the equipartition principle does not hold for an inelastic system, and some provide more general results. Also the earliest constitutive model of Jenkins & Mancini [1] took energy non-equipartition into account (in the dense limit), by incorporating first-order corrections in the fluctuation energy difference. The theoretical studies have been complemented by both computer simulations [11–14] and laboratory experiments [15,16], which verifed the breakdown of the equipartition principle for granular mixtures. All these works collectively showed that even though the inelasticity is responsible for the *onset* of energy non-equipartition, it is the *mass-disparity* which strongly amplifies its magnitude.

It is important to know the range of validity of any constitutive model in terms of all the control parameters as well as the validity of some of its underlying assumptions if one wishes to use it for predictive purposes. For example, if the effect of the non-equiparton of energy on the transport coefficients (pressure, viscosity, thermal conductivity, etc.) is minimal, one could still rely on the effective mixture models with equipartition assumption.

Here we show, using the event-driven simulation of a sheared binary granular mixture, that the breakdown of the equipartition principle leads to certain interesting behaviour of its transport coefficients (pressure and shear viscosity). However, the *effective mixture-theory*, with the equipartition assumption, fails to predict the qualitative behaviour of pressure and viscosity in such situations.

2 Simulation details

We consider a collection of smooth inelastic hard-disks in a square box of size $\tilde{L}$ under uniform shear flow — let $\tilde{x}$ and $\tilde{y}$ be the streamwise and transverse directions, respectively, with the origin of the coordinate-frame being positioned at the centre of the box. (Note that the dimensional quantities are denoted by tildes, while their nondimensional counterparts lack it.) Let the diameter and the mass of the particle i be $\tilde{d}_i$ and $\tilde{m}_i$ $(i = l, s)$, respectively, with the suffix l or s denoting the species of *larger/smaller* mass, respectively. That the particles are dissipative is taken into account through the following relation for the pre- and post-collisional velocities:

$$\mathbf{k}\cdot\tilde{\mathbf{c}}'_{ji} = -e_{ij}(\mathbf{k}\cdot\tilde{\mathbf{c}}_{ji}), \qquad (1)$$

with e_{ij} being the coefficient of normal restitution for collisions between particles i and j. Here $\tilde{\mathbf{c}}_{ji} = \tilde{\mathbf{c}}_j - \tilde{\mathbf{c}}_i$ is the relative velocity, and $\mathbf{k}_{ji} = \mathbf{k}$ the unit vector directed from the center of the particle j to that of particle i. We used the familiar Lees-Edwards boundary condition [17] to attain the state of uniform shear flow (USF). Overall, this represents an *extended doubly-periodic* system where the periodicity in the transverse direction is in the local Lagrangian frame.

The disks are initially placed randomly in the box, and the initial velocity field is composed of the uniform shear

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and a small Gaussian random part. Given the initial position and velocities of the particles, an event-driven algorithm is used to simulate instantaneous binary collisions. At the statistical steady-state of the uniform shear flow, the fluctuation kinetic energy saturates to a constant value after the initial transients, a consequence of the balance between the shear work and the collisional dissipation. After reaching such a steady-state, the simulation is then allowed to run for another 20000 collisions per particle to gather data to calculate the pressure, shear viscosity and granular energy.

To obtain pressure and shear viscosity from simulations, we have to calculate the macroscopic stress which is composed of two different parts, kinetic stress and collisional stress, each being a byproduct of a separate mode of momemtum transport at the microscopic level. While the transport of momentum as a particle moves through the system, carrying the momentum of its motion, is responsible for the 'kinetic' mode of stress, the direct interparticle collisions generate its 'collisional' component. The total stress tensor is thus calculated from

$$\tilde{\mathbf{P}} = \sum_{i=l}^{s}(\tilde{\mathbf{P}}_i^k + \tilde{\mathbf{P}}_i^c) = \sum_{i=l}^{s}\left[\frac{1}{N_i}\sum_{i=1,N_i}\tilde{\rho}_i\nu_i\tilde{\mathbf{C}}_i\tilde{\mathbf{C}}_i + \frac{1}{2\tilde{L}^2\tau_d}\sum_{collisions}(\tilde{d}_i+\tilde{d}_j)(\tilde{\mathbf{I}}_{ij}\otimes\mathbf{k})\right] \quad (2)$$

where $\tilde{\rho}_i$ and ν_i are the material density and the volume fraction of species i, $\tilde{\mathbf{C}}_i = \tilde{\mathbf{c}}_i - \tilde{u}$ is the peculiar velocity and $\tilde{\mathbf{I}}_{ij}$ is the collisional impulse. Note that for the collisional stress, $\tilde{\mathbf{P}}_i^c$, the sum is taken over all collisions during the averaging time window τ_d. For the uniform shear flow, all these quantities (except the streamwise velocity which varies linearly with the transverse coordinate) are uniform in the computational box, which in turn allows us to take averages over the whole computational box, as made explicit in Eq. (2).

The pressure, $\tilde{p}$, is then calculated from the isotropic part of the stress $\tilde{\mathbf{P}}$. From the off-diagonal components of the pressure deviator, $\tilde{\Pi} = \tilde{\mathbf{P}} - \tilde{p}\mathbf{1}$, we can calculate *shear viscosity* which relates the shear stress to the shear rate:

$$\tilde{\mu} = \tilde{\Pi}_{xy}/\frac{\mathrm{d}\tilde{u}}{\mathrm{d}\tilde{y}} \quad (3)$$

Both pressure and viscosity are nondimensionalized by $\tilde{\rho}_l\tilde{d}_l^2\tilde{\gamma}^2$ and $\tilde{\rho}_l\tilde{d}_l^2\tilde{\gamma}$, respectively, with $\tilde{\gamma}$ being the imposed shear rate. Granular energy, which is a measure of the random motion of the particles, may be obtained from the trace of the kinetic part of the stress tensor, and the *species* granular energy is calculated from the following expression:

$$T_i = \frac{\tilde{T}_i}{\tilde{m}_l\tilde{d}_l^2\tilde{\gamma}^2} = \left(\frac{1}{2d_l^2}\right)\left[\frac{1}{N_i}\sum_{i=1,N_i} m_i\mathbf{C}_i\mathbf{C}_i\right] \quad (4)$$

The *mixture* granular energy is $T = \sum_{i=l,s}\xi_i T_i$, where $\xi_i = N_i/N$ is the number fraction of species i.

As mentioned before, we consider the *equal-size* ($d_l = d_s$) bidisperse mixture, characterized only by density or mass-disparity. The total number of particles and the imposed shear rate γ were fixed at 1024 and 1, respectively, and we have checked that the reported results do not depend on the system-size and the shear rate [13]. Thus, there are four dimensionless control parameters: the total solids volume fraction (ν), the relative volume fraction of heavier particles ($\chi = \nu_l/\nu$), the mass ratio ($R_m = m_l/m_s$), and the coefficient of normal restitution (e). The detailed results will be presented elsewhere. Below, a set of numerical results is presented to probe the validity of the kinetic theory constitutive model with the equipartition assumption and a simple extension based on the species energy ratio is proposed.

3 Results and discussion

First we recall the standard form of the Newtonian stress tensor

$$\mathbf{P} = p\mathbf{1} - 2\mu\mathbf{S}, \quad (5)$$

where $\mathbf{S}$ is the deviatoric part of the shear-rate tensor. The effective mixture theory [4,2] with the equipartition assumption, postulates the following expressions for pressure and shear viscosity:

$$p = T\sum_{i=l}^{s} f_{pi} \quad \text{and} \quad \mu = \sqrt{T}\sum_{i=l}^{s} f_{\mu i}, \quad (6)$$

where $T = \sum_{i=l,s}\xi_i T_i$ is called the mixture temperature. Similarly, following Jenkins & Mancini [1,2], the constitutive expression for the collisional dissipation rate can be written as:

$$\mathcal{D} = T^{3/2}\sum_{i=l}^{s} f_{\mathcal{D}i}. \quad (7)$$

The functions, f_{pi}, $f_{\mu i}$ and $f_{\mathcal{D}i}$ depend on the density ratio, size-ratio, mass ratio, inelasticity, and the radial distribution function, the explicit forms of which may be obtained from the Enskog theory of binary mixtures [2,6].

For the steady ($\frac{\partial}{\partial t}(.) = 0$), fully developed ($\frac{\partial}{\partial x}(.) = 0$) plane shear flow of a binary granular mixture, it is easy to verify that a linear streamwise velocity profile along with constant density and constant granular energy satisfies the balance equations [13]. Thus, the mean fields are given by

$$\left.\begin{array}{l} \phi = \sum_{i=l}^{s}\phi_i \ = \ \text{const.} \\ T = \sum_{i=l}^{s}\xi_i T_i \ = \ \text{const.} \\ \mathbf{u} \equiv (u,v)^T \ = \ (y,0)^T \end{array}\right\} \quad (8)$$

An explicit expression for T can be obtained from the energy balance equation, by equating the production term due to shear-work ($-\mathbf{P}{:}\nabla\mathbf{u}$) with the collisional dissipation rate ($\tilde{\mathcal{D}}$):

$$T = \frac{\sum_{i=l}^{s} f_{\mu i}}{\sum_{i=l}^{s} f_{\mathcal{D}i}}. \quad (9)$$

Figure 1 shows the variation of the ratio between the two *species* granular energies, T_l/T_s, with the mass ratio, $R_m = m_l/m_s$. The parameter values are set to $\nu = 0.1$, $\chi = 0.5$ and $e = e_{ij} = 0.9$. The symbols represent our simulation data– clearly, the granular energy is *unequally* partitioned between the two species, and the degree of this non-equipartition increases with the mass-ratio. The

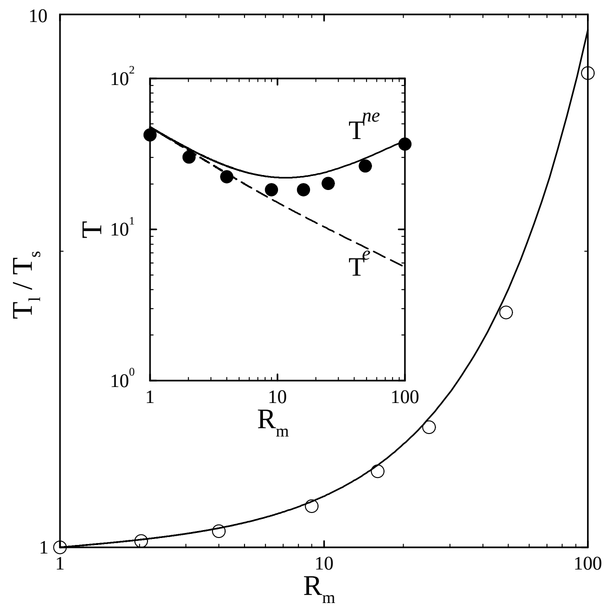

Fig. 1. Variation of the ratio of the species granular energies, T_l/T_s, with the mass ratio for $\nu = 0.1$, $\chi = 0.5$ and $e = 0.9$. The solid line is the prediction of Barrat & Trizac (2002). The inset shows the comparison of mixture granular energy between simulation and theory: solid line is the model prediction, T^{ne}, with nonequipartion of energy, and the dashed line, T^e, with equipartition assumption.

solid line in this Fig. is due to Barrat & Trizac [9] who obtained an implicit nonlinear expression for the granular energy ratio, $R_T = T_l/T_s$, for a driven granular gas:

$$C_1 R_T^{3/2} + C_2 \left(1 + \frac{m_s}{m_l} R_T\right)^{3/2} + C_3 \left(1 + \frac{m_s}{m_l} R_T\right)^{1/2} (R_T - 1) + C_4 \ = \ 0, \qquad (10)$$

with

$$C_1 = 2^{d-1}(1 - e_{ll}^2) R_{sl}^d \nu_l g_{ll} \left(\frac{m_s}{m_l}\right)^{3/2}$$
$$C_2 = \sqrt{2}(1 - e_{ls}^2)(1 + R_{sl})^{d-1} \left(\nu_s M_{sl}^2 - \nu_l R_{ls}^d M_{ls}^2\right) g_{ls}$$
$$C_3 = 2\sqrt{2}(1 + e_{ls})(1 + R_{sl})^{d-1} M_{sl} \left(\nu_s M_{sl} + \nu_l R_{ls}^d M_{ls}\right) g_{ls}$$
$$C_4 = -2^{d-1}(1 - e_{ss}^2) R_{ls}^{d+1} \nu_s g_{ss}.$$

Here g_{ij} is the radial distribution function at contact, d is the dimensionality of the problem, $M_{ij} = m_i/(m_i + m_j)$ and $R_{ij} = d_i/d_j \equiv 1$. Overall, there is a good agreement between simulation and theory. (Strictly speaking, the expression for T_l/T_s for the uniform shear flow should be obtained by equating the shear-work and the dissipation rate for the individual species. Since we do not have an exact expression for the shear viscosity of a binary mixture, with $T_l \neq T_s$, we have chosen the expression of Barrat & Trizac.) The inset in Fig. 1 shows the corresponding variation of the *mixture* granular energy T with the mass ratio. While our simulation data shows an interesting nonmonotonic behaviour for T, the predictions of Eq. (9), given by the dashed line, shows that $T = T^e$ decays monotonically.

Figure 2 shows the variations of pressure and viscosity and their partial components with the mass ratio. The overall behaviour looks similar to that of the granular energy. It is noteworthy that at large mass-disparities the major contribution to both pressure and viscosity comes from the heavier particles only. The theoretical predictions from Eq. (6) (not shown on the graph) suggest a monotonically decreasing behaviour for p and μ and their partial components, quite contrary to our simulations.

Now let us postulate the constitutive relations for p, μ and $\mathcal{D}$ allowing energy non-equipartition in a simple way:

$$p = \sum_{i=l}^{s} f_{pi}(T_l/T_s, ...)T_i,$$

$$\mu = \sum_{i=l}^{s} f_{\mu i}(T_l/T_s, ...)\sqrt{T_i},$$

$$\mathcal{D} = \sum_{i=l}^{s} f_{\mathcal{D}i}(T_l/T_s, ...)T_i^{3/2}$$

(To understand the above functional forms, we consider the kinetic-part of the pressure, p^k. Assuming that the singlet distribution function of species i is a Maxwellian at its own temperature, it can be verified [1] that $p^k = \sum_{i=l,s} \nu_i T_i$. Similarly, we can obtain an expression for the collisional part of the pressure, p^c. The details of these functional forms will appear in a forthcoming publication.) Note that the functions,f_{pi}, $f_{\mu i}$ and $f_{\mathcal{D}i}$ now depend additionally on T_l/T_s. The expression for $f_{\mathcal{D}i}(T_l/T_s, ...)$ can be obtained by assuming Maxwellian distribution functions for each species. Since we do not have exact expression for $f_{\mu i}(T_l/T_s, ...)$, we have taken it simply from Willits & Arnarson [6]. (This choice does not influence the predictions at low densities.) The granular energy can again be calculated from Eq. (9), by knowing the energy ratio from Barrat & Trizac [9].

The predictions of this simplified model for T, p and μ are shown in figures 1 and 2. This model is able to capture the trend of our data and the overall agreement is good.

Lastly, the reason for such nonmonotonic behaviour of pressure and viscosity can be understood by recalling their variation with density for a sheared *monodisperse* granular system. Typically, the variations of both p and μ with density follow U-shaped curves, with minimums occuring at a density of $\nu \approx 0.3$. Since the lighter particles do not contribute to transport properties due to their *low-mobilities* at large mass-ratios, the system would behave as if it were composed of *only* heavier particles with an effective *lower* density, depending on the relative volume fraction χ. Hence both pressure and viscosity would eventually increase in the same limit.

4 Conclusions

The interesting finding from our simulation data on pressure and viscosity is their *non-monotonic* behaviour with the mass-ratio, whereas the theoretical predictions with the equipartition assumption suggest a *monotonic* behaviour. This is directly related to the *violation* of the equipartition principle at large mass-ratios for which the mix-

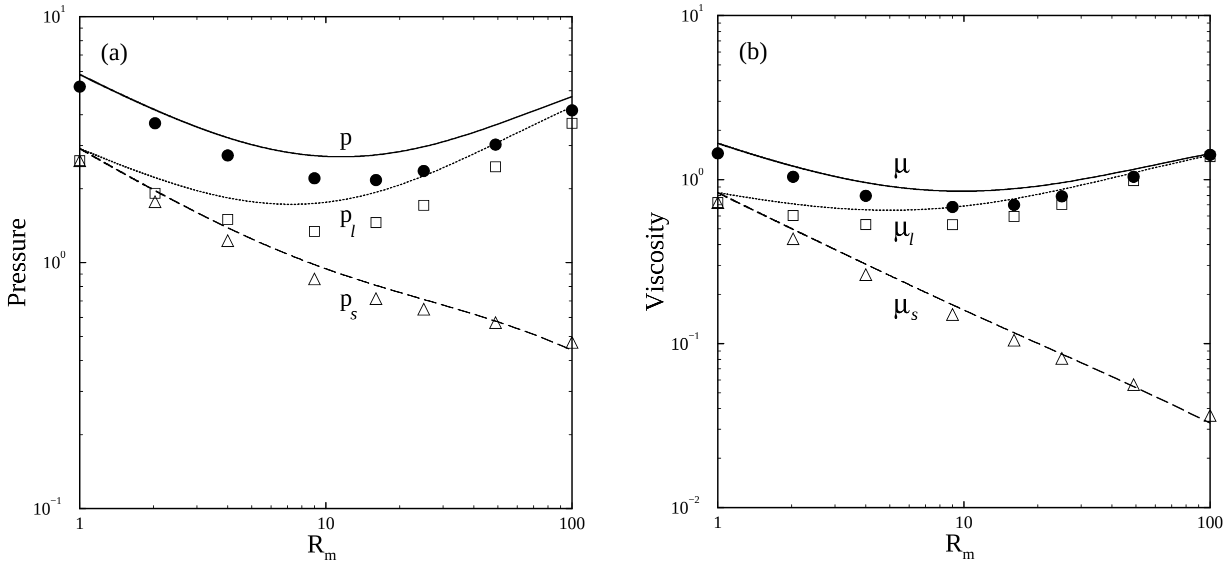

Fig. 2. Variations of (*a*) pressure, (*b*) viscosity and their partial components, with the mass-ratio $R_m = m_l/m_s$; parameter values as in figure 1. Symbols denote simulation data and the lines the model predictions.

ture effectively behaves like a lower-density system. Even though the example we have chosen is very simple-minded, it demonstrates that a proper constitutive model for a granular mixture must incorporate the effect of non-equipartition of granular energy. An interesting practical application is the tuning of flow properties by adding equal-size lighter particles to the system. More interesting results can be expected when both mass- and size-ratios are tuned [13].

References

1. J. T. Jenkins and F. Mancini. Balance laws and constitutive relations for plane flows of a dense, binary mixture of smooth, nearly elastic, circular disks. *J. Appl. Mech.*, 54:27, 1987.
2. J. T. Jenkins and F. Mancini. Kinetic theory for binary mixtures of smooth, nearly elastic spheres. *Phys. Fluids A*, 1:2050, 1989.
3. S. Chapman and T. G. Cowling. *The Mathematical Theory of Nonuniform Gases.* Cambridge Univ. Press, London, 1970.
4. M. López de Haro and E. D. G. Cohen and J. M. Kincaid. The Enskog theory for multicomponent mixtures. I. Linear transport theory. *J. Chem. Phys.*, 78:2746, 1983.
5. B. Ö. Arnarson and J. T. Willits. Thermal diffusion in binary mixture of smooth, nearly elastic spheres with and without gravity. *Phys. Fluids*, 10:1324, 1998.
6. J. T. Willits and B. Ö. Arnarson. Kinetic theory of a binary mixture of nearly elastic disks. *Phys. Fluids*, 11:3116, 1999.
7. P. A. Martin and J. Piasecki. Thermalization of a particle by dissipative collisions. *Europhys. Lett.* 46:613, 1999.
8. V. Garzo and J. W. Dufty. Homogeneous cooling state for a granular mixture. *Phys. Rev. E*, 60:5706, 1999.
9. A. Barrat and E. Trizac. Lack of energy equipartition in homogeneous heated binary granular mixtures. *Granular Matter*, 4(2):XXX, 2002.
10. L. Trujillo and H. J. Herrmann. Hydrodynamic model for particle size segregation in granular media. *Preprint*, 2002.
11. S. Luding, O. Strauss and S. McNamara. Segregation of polydisperse granular media in the presence of a temperature gradient. In A.D. Rosato and D.L. Blackmore, editors, *IUTAM Symposium on Segregation in Granular Flows*, pages 297-304, Dordrecht, 2000, Kluwer Academic Press.
12. S. Luding and O. Strauss. The equation of state of polydisperse granular gases. In T. Pöschel and S. Luding, editors, *Granular Gases*, pages 389-409, Berlin, 2001. Springer.
13. M. Alam and S. Luding. Rheology of bidisperse granular media: a computer simulation study. *Preprint*, 2002.
14. J. M. Montanero and V. Garzo. Monte carlo simulation of the homogeneous cooling state for a granular mixture. *Granular Matter*, 4(1):17, 2002.
15. R. D. Wildman and D. J. Parkar. Energy nonequipartition in a vibrated granular gas mixture. *Phys. Rev. Lett.*, 88:064301, 2002.
16. K. Feitosa and N. Menon. Breakdown of energy equipartition in a 2D binary vibrated granular gas. *Phys. Rev. Lett.*, 88:198301-1, 2002.
17. A. W. Lees and S. F. Edwards. The computer study of transport processes under extreme conditions. *J. Phys. C*, 5(6):1921, 1972.