On the cooling law of a non-dilute granular gas

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The cooling law of a granular gas was investigated using a three-dimensional MD simulation code, which allowed us to include both inelasticity and frictional effects of the particle contacts. It was found that the kinetic energy decays in time as $E(t) \sim t^{-n}$; the exponent n of the cooling law changes significantly with the solid fraction, α, and the coefficient of restitution, ϵ. For dilute gases, for times greater than t_c, we found that $n \approx 1$, in agreement with the results reported by Nie *et al.* [10]. As α and/or ϵ increase, the cooling coefficient increases to an asymptotic value of $n \approx 2.2$, which is slightly higher than the prediction made by Haff [3]. We interpret this increase in the cooling exponent as a possible re-homogenization of the granular state.

Keywords: Granular gas; cooling; Haff's law.

Estudiamos la ley de enfriamiento de un gas granular de manera computacional utilizando un programa de tipo MD, el cual permite considerar tanto la inelasticidad como la rugosidad de las partículas. Encontramos que la energía cinética del sistema decae en el tiempo de acuerdo a $E(t) \sim t^{-n}$; el exponente n de enfriamiento cambia de manera significativa para cambios en la fracción sólida del sistema α, y el coeficiente de restitución, ϵ, que caracteriza la inelasticidad de los choques. Para gases diluidos, para tiempos mayores que t_c, encontramos que $n \approx 1$, lo cual concuerda con lo reportado por Nie *et al.* [10]. Sin embargo, conforme α y/o ϵ se incrementan, el exponente de enfriamiento crece hasta alcanzar un valor asintótico de $n \approx 2.2$, que es un poco mas grande que el valor predicho por Haff [3]. Especulamos que este incremento de la tasa de enfriamiento se debe a la rehomogeneización del sistema granular.

Descriptores: Gas granular; enfriamiento; ley de Haff.

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1. Introduction

The understanding of rapid-dilute granular flows has advanced significantly in the last few years [1]. For this particular configuration, the system is amenable to theoretical treatment using the kinetic theory of gases [2]. Also, such systems have been extensively studied by means of molecular dynamics computer simulations, also known as discrete element simulations (see also Ref. 1). However, the quantitative characterization of many features of rapid granular flows remain yet to be fully resolved (clustering regime, typical length and velocity scales, particle velocity distributions, etc., to name just a few).

Of particular interest, due to its simplicity, is the so-called homogeneous cooling state (HCS): the *granular temperature* of a granular gas consisting of homogeneously distributed particles with zero mean velocity will *cool off* in time as a result of the inelasticity of the collisions. The granular temperature is the mean kinetic energy of the system.

A prediction for the cooling rate of a granular gas was first reported by Haff [3], and has been studied by many others since then [4–11]. By considering that the kinetic energy of the gas is dissipated solely by collisions, the energy conservation equation reduces to

$$\frac{\partial}{\partial t}\left(\frac{1}{2}\alpha\rho_p\langle v^2\rangle\right) = (\Delta E_c)\dot{C}N, \qquad (1)$$

where α is the particle solid fraction, ρ_p is the particle density, $\langle v^2\rangle$ is the variance of the particle velocity, ΔE_c is the energy dissipated during each collision, $\dot{C}$ is the collision rate and N is the number density. The details of the derivation of this equation can be found in the original reference. The energy dissipation per collision can be written as $\Delta E_c \approx -(1-\epsilon^2)(1/2)m\langle v^2\rangle$, where ϵ is the coefficient of normal restitution. For a dilute gas of equal particles of diameter d, the collision rate is $\dot{C} = N(\pi d^2)\sqrt{\langle v^2\rangle}$. The particle mass m can also be written as $m = \rho_p(\pi/6)d^3$. Similarly, the number density N can be written in terms of the particle volume fraction, α, as: $\alpha = N(\pi/6)d^3$. Hence, Eq. (1) can be written as

$$\frac{\partial}{\partial t}\left(\alpha\langle v^2\rangle\right) = -\frac{6}{d}(1-\epsilon^2)(\alpha^2\langle v^2\rangle\sqrt{\langle v^2\rangle}). \qquad (2)$$

Haff solved this equation by considering that α was constant, leading to

$$\frac{\langle v^2\rangle}{\langle v^2\rangle_o} = \left(1 + \frac{3}{d}(1-\epsilon^2)\sqrt{\langle v^2\rangle_o}\alpha t\right)^{-2}, \qquad (3)$$

which implies that the kinetic energy of the system decays as $E(t) \sim t^{-2}$. It has been shown [8, 10] that the initial decay of kinetic energy is predicted correctly by Haff's cooling law. From Eq. (1), it can be inferred that the characteristic time for which the distribution of particles is expected to remain homogeneous is proportional to $(1-\epsilon^2)\sqrt{\langle v^2\rangle_o}/d$. As time progresses, the assumption that

α remains constant no longer holds, due to the formation of clusters [5, 9, 11, 12]. Nie *et al.* [10] showed that, for 2-D dilute systems ($\alpha = 0.071$) the kinetic energy decays as $E(t) \sim t^{-1}$. For dense systems, which have not been fully explored to date, the evolution of particle cluster leads to a different cooling behavior. Clearly, for dense systems, Eq. (1) would have to be solved simultaneously with a concentration evolution equation,

$$\frac{\partial \alpha}{\partial t} + \nabla(\langle \alpha \mathbf{v} \rangle) = 0. \tag{4}$$

Since the mathematical solution to this system is not yet possible, we opted for numerical experimentation to investigate the behavior of non-dilute cooling granular gases.

In this paper, we report the variation of the cooling rate exponent found by MD numerical simulations. In particular, we explore the influence of the contact properties of the collisions (normal coefficient of restitution, ϵ, and friction coefficient, μ) and the concentration of the system (particle volume fraction, α).

Simulations of the granular system consisted of 1000 spheres randomly placed in a cubic box, at a fixed homogeneous initial solid fraction (α=0.05, 0.1, 0.2 and 0.4), with initial velocities chosen from a Gaussian distribution. Therefore, with the definition of the solid fraction given some paragraphs above, we can also find the volume of the simulation cell ($V = L^3$) used for each α, $V = M(\pi/6)d^3/\alpha$, where M is the number of spheres. Therefore, the size simulation cells were L = 21.878d, 17.365d, 13.783d and 10.939d for α=0.05, 0.1, 0.2 and 0.4, respectively. Thus, the MD simulations were performed by solving the equations of motion of all the particles in the system.

Moreover, the simulation parameters were chosen to be those of particles commonly used in experimental research, *i.e.* the sphere radius of r=0.5$\times 10^{-3}$m and mass m= 1.308$\times 10^{-6}$ kg using different restitution (ϵ= 0.49, 0.85 and 0.97) and friction (μ= 0.0, 0.1, 0.2) coefficients. A few tests were performed for 5000 and 10000 particles to check the validity of the results; no significant differences were observed.

All simulations were performed for 3$\times 10^6$ δt (δt = 4$\times 10^{-7}$ s). The code used in this study considers particle contacts with both inelasticity and frictional effects. The contact forces are modelled for both the normal and tangential directions. For the normal direction the linear hysteretic spring model proposed by Walton and Braun [14] was used, which accounts for the collision energy loss using a spring with two different stiffnesses. The loading stiffness is chosen to match Hertzian contact parameters; the unloading stiffness is calculated from the loading stiffness and the coefficient of restitution. For the tangential direction, a linear spring in series with the Coulomb sliding friction element model was used as proposed by Cundall and Strack [13]. In this manner it was possible to test the effects of both inelasticity and friction on the behavior of cooling granular gases.

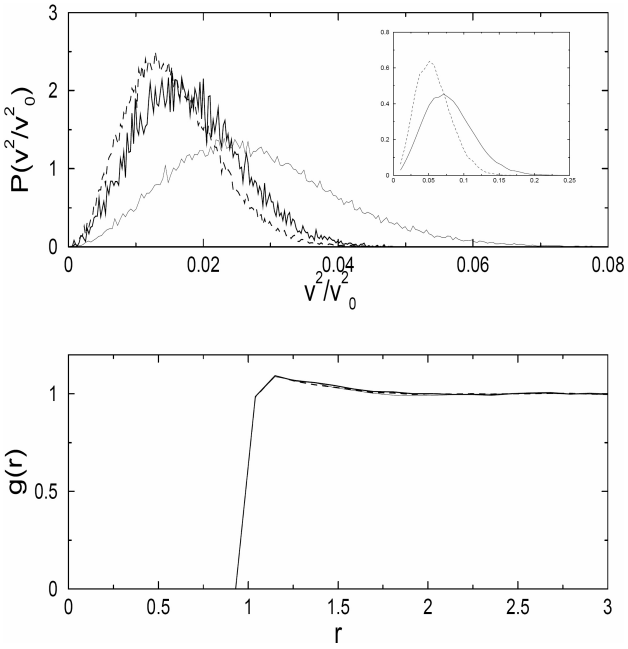

FIGURE 1. Velocity distributions at different times (top) (the inset shows distributions at short times, see the x-scale difference) with their respective pair distribution functions, $g(r)$ (bottom). The results are for ϵ = 0.85 and α = 0.05. Each graph is the average over 2$\times 10^5$ δt after 1.4$\times 10^6$ δt (light solid line), 2$\times 10^6$ δt (dark solid line) and 2.8$\times 10^6$ δt (dashed line). For the inset also is the average over 2$\times 10^5$ δt after 2$\times 10^5$ δt (solid line) and 4$\times 10^5$ δt (dashed line).

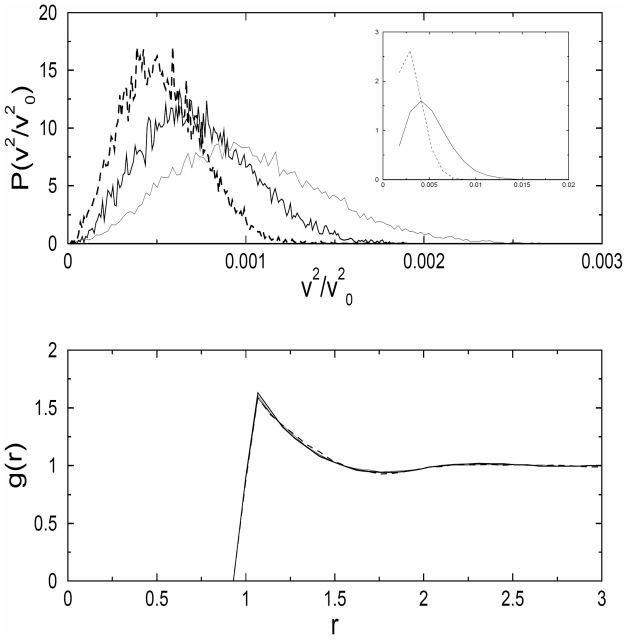

FIGURE 2. The same as Fig. 1 for ϵ = 0.85 α = 0.2.

2. Results

Figures 1, 2, and 3 show typical velocity distributions of the particles along the simulation time. Each distribution repre-

sents the average over 2×10^5 δt independent blocks. It can be observed that the velocity distribution becomes sharper at low velocities. The pair distribution function, $g(r)$, was also calculated in each block, for all the times tested (*i.e.* long times).

Since the pair distribution function did not evolve with time, it can be argued that particles are already in the clustering regime, as pointed out by Nie *et al.*; however, it must be noted that the observed $g(r)$-structure is *weak*. As the volume fraction increases, a second peak appears around two particle diameters (Fig. 3), *i.e.* the $g(r)$ presents a structure more similar to that of a dilute liquid.

Figure 4 shows typical graphs of $E(t)/E_{k0}$ as a function of time for different restitution coefficients and solid fractions where E_{k0} is the initial kinetic energy. As discussed by

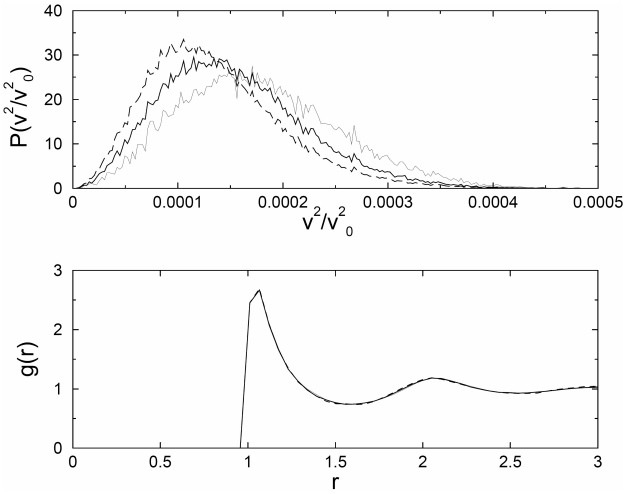

FIGURE 3. The same as Fig. 1 for ϵ = 0.85 α = 0.4. Each graph is the average over 2×10^5 δt after 1×10^6 δt (light solid line), 1.2×10^6 δt (dark solid line) and 1.4×10^6 δt (dashed line).

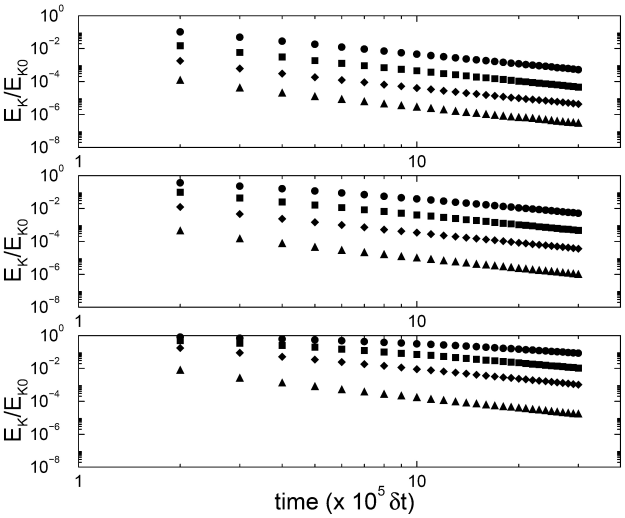

FIGURE 4. Dimensionless kinetic energy as a function of time. Solid fractions of α = 0.05 (●), 0.1 (■), 0.2 (♦) and 0.4 (▲) for restitution coefficients ϵ = 0.49 (top) 0.85 (middle) and 0.97 (bottom).

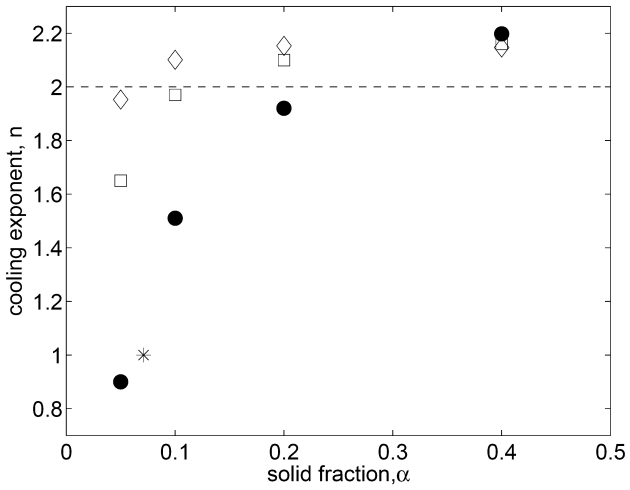

FIGURE 5. The cooling exponent n as a function of solid fraction, α, for a range of values of the coefficient of restitution: (♢), ϵ_n = 0.49; (□), ϵ_n = 0.85; (●), ϵ_n = 0.97. For all simulations the friction coefficient is $\mu = 0.1$. The dashed line shows the prediction of Haff [3], $n = 2$. The asterisk (*) shows the result of [10].

several authors before, the energy decayed algebraically with time as

$$\frac{E(t)}{E_{k0}} \sim t^{-n}. \tag{5}$$

Clearly, the rate of energy decay increases with the solid fraction and also the restitution coefficient. Simulations were also performed for friction coefficients of μ =0.0, 0.1 and 0.2; the results (not shown) were nearly the same for all the cases. Hence, for these systems the main contribution on cooling comes from the normal collisions between particles and the friction forces between particles can be neglected.

From the results shown in Fig. 4, the cooling exponent, n, was calculated by fitting an algebraic function to the different curves. The results are shown in Fig. 5, as a function of the particle concentration and for several values of the restitution coefficient. At low solid fractions, α = 0.05, the cooling exponent is lower than 2, regardless of the restitution coefficient. However, for ϵ = 0.97, the exponent is nearly one (n = 0.90). For a 2-dimensional system, at a low solid fraction, Nie *et al.* [10] found a cooling exponent of n = 1.

As the solid fraction increases, the cooling exponent also increases to reach an asymptotic value $n \approx 2.2$. Note that this value is closer to that Haff's law [3].

These results indicate that as α increases the granular gas dissipates its energy at a rate which is closer to that predicted for a homogeneous state. It has been claimed by others that the appearance of clusters reduces the cooling rate. Based on our results, we can argue that cluster reduction of the cooling rate may only be valid for dilute gases. For non-dilute gases, the inhomogeneities in the particle concentration may not be as strong as those in the dilute case. It is also important to note that most of the studies that have reported slower cooling rates than Haff's prediction are for dilute 2D gases [8,10].

Since our results are 3D, we can also argue that, as the dimensionality of the system increases, the cooling rate also increases: for a 1D gas, the cooling rate has been reported to be $n = 2/3$ [15]; for 2D, Nie *et al.* [10] report a value of $n = 1$.

In summary, our MD simulations performed on frictional inelastic 3D granular gases showed that the cooling rate increases with the particle volume fraction, reaching values which are slightly higher that those predicted for homogeneous gases. This is an indication that, for denser 3D gases, the system become more homogeneous. We also found that the frictional properties of the particle contacts have a negligible effect on the cooling rate of the granular gas. A more in-depth investigation should be performed to further investigate the homogenization of the particle distribution for non-dilute granular gases.

Acknowledgments

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