KINETIC THEORY OF GRANULAR BINARY MIXTURES

Vicente Garzó

Departamento de Física, Universidad de Extremadura, Badajoz, Spain

J.W. Dufty (Univ. Florida)

J. M. Montanero (UEx)

Temperature in non-equilibrium systems, September, 18-19, 2008, Barcelona

OUTLINE

1. Introduction

2. Granular binary mixtures. Inelastic Boltzmann equation

3. Homogeneous cooling state. Energy nonequipartition

4. Sheared granular mixtures

5. Summary and conclusions

INTRODUCTION

Behaviour of granular systems under many conditions exhibit a great similarity to ordinary fluids

Rapid flow conditions: hydrodynamic-like type equations.Good example of a system which is inherently in *non-equilibrium*

Dominant transfer of momentum and energy is through ***binary inelastic*** collisions. Subtle modifications of the usual macroscopic balance equations

To isolate collisional dissipation: *idealized* microscopic model

Smooth hard spheres
with *inelastic* collisions

$$\mathbf{V}_{12}^{*} \cdot \widehat{\boldsymbol{\sigma}} = -\alpha \mathbf{V}_{12} \cdot \widehat{\boldsymbol{\sigma}}$$

Coefficient of restitution

$$0 < \alpha \leq 1$$

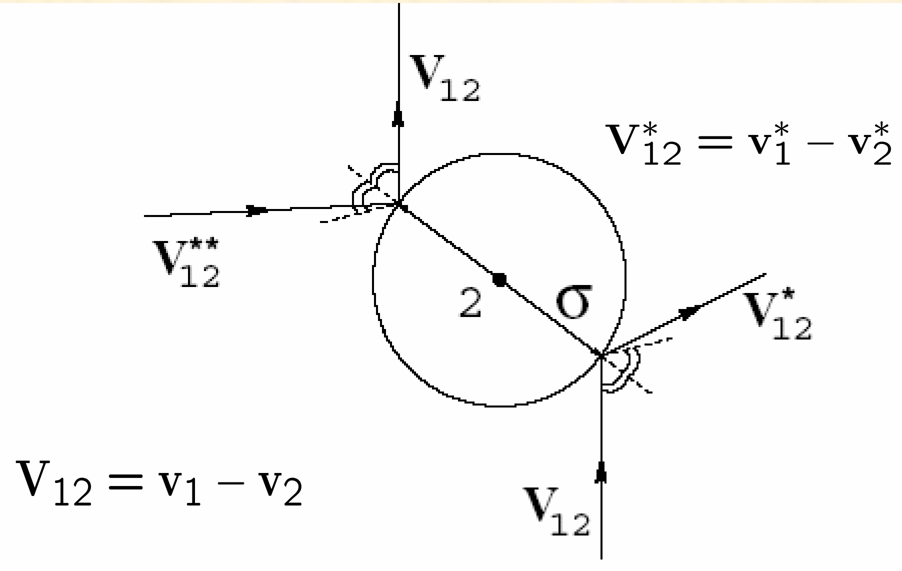


FIG. 1: Sketch of inelastic collisions (after T.P.C. van Noije & M.H. Ernst).

Direct collision

$$\mathbf{v}_1^{*} = \mathbf{v}_1 - \frac{1}{2}(1+\alpha)\,(\widehat{\boldsymbol{\sigma}} \cdot \mathbf{V}_{12})\widehat{\boldsymbol{\sigma}}$$

$$\mathbf{v}_2^{*} = \mathbf{v}_2 + \frac{1}{2}(1+\alpha)\,(\widehat{\boldsymbol{\sigma}} \cdot \mathbf{V}_{12})\widehat{\boldsymbol{\sigma}}$$

Momentum conservation

$$\mathbf{v}_1 + \mathbf{v}_2 = \mathbf{v}_1^* + \mathbf{v}_2^*$$

Collisional energy change

$$\Delta E = \frac{1}{2} m \left(v_1^{*2} + v_2^{*2} - v_1^2 - v_2^2 \right) = -\frac{m}{4} (1 - \alpha^2) (\mathbf{V}_{12} \cdot \hat{\boldsymbol{\sigma}})^2$$

Very **simple** model that *captures* many properties of granular flows, especially those associated with dissipation

KINETIC DESCRIPTION

One-particle velocity distribution function (vdf)

$$f(\mathbf{r},\mathbf{v},t)d\mathbf{r}d\mathbf{v} \longrightarrow$$

Average *number of particles* wich at *t* lie in r+*d*r and move with **v**+*d***v**

Boltzmann kinetic equation

- ***Dilute*** gas (binary collisions)
- ***Molecular chaos*** (no velocity correlations)

$$(\partial_t + \mathbf{v}\cdot\nabla)\, f(\mathbf{v}) = J\left[\mathbf{v}|f(t), f(t)\right]$$

$$J[f,f] = \sigma^{d-1}\int d\mathbf{v}_2 \int d\widehat{\boldsymbol{\sigma}}\, \Theta(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g})(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g})\left[\alpha^{-2} f(\mathbf{v}_1')f(\mathbf{v}_2') - f(\mathbf{v}_1)f(\mathbf{v}_2)\right]$$

Scattering rules:

$$\mathbf{V}_{12} \equiv \mathbf{g}$$

$$\mathbf{v}_1' = \mathbf{v}_1 - \frac{1}{2}\left(1+\alpha^{-1}\right)(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g})\widehat{\boldsymbol{\sigma}}$$

$$\mathbf{v}_2' = \mathbf{v}_2 + \frac{1}{2}\left(1+\alpha^{-1}\right)(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g})\widehat{\boldsymbol{\sigma}}$$

Differences with respect to the usual BE:

Presence of α^{-2} in the gain term and collision rules

Binary granular *mixtures*. Boltzmann description

Mechanical parameters: $\{m_1, m_2, \sigma_1, \sigma_2, \alpha_{11}, \alpha_{22}, \alpha_{12}\}$

Extension of the BE to the *multicomponent* case: $f_i(\mathbf{r}, \mathbf{v}, t)$

$$(\partial_t + \mathbf{v}\cdot\nabla)\, f_i(\mathbf{v}) = \sum_j J_{ij}\left[\mathbf{v}|f_i(t), f_j(t)\right]$$

$$J_{ij}[f_i, f_j] = \sigma_{ij}^{d-1}\int d\mathbf{v}_2 \int d\widehat{\boldsymbol{\sigma}}\, \Theta(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g})(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g})\left[\alpha_{ij}^{-2} f_i(\mathbf{v}_1')f_j(\mathbf{v}_2') - f_i(\mathbf{v}_1)f_j(\mathbf{v}_2)\right]$$

$$\sigma_{ij} = \frac{\sigma_i + \sigma_j}{2}$$

Collision rules:

$$\mathbf{v}_1' = \mathbf{v}_1 - \mu_{ji}\left(1+\alpha_{ij}^{-1}\right)(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g})\widehat{\boldsymbol{\sigma}}$$

$$\mathbf{v}_2' = \mathbf{v}_2 + \mu_{ij}\left(1+\alpha_{ij}^{-1}\right)(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g})\widehat{\boldsymbol{\sigma}}$$

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

Hydrodynamic fields

$$n_i(\mathbf{r},t) = \int d\mathbf{v}\, f_i(\mathbf{r},\mathbf{v},t)$$

$$\mathbf{U}(\mathbf{r},t) = \frac{1}{\rho(\mathbf{r},t)}\sum_i \int d\mathbf{v}\, m_i \mathbf{v} f_i(\mathbf{r},\mathbf{v},t)$$

Granular temperature

$$T(\mathbf{r},t) = \frac{1}{n(\mathbf{r},t)}\sum_i \int d\mathbf{v}\frac{m_i}{d}(\mathbf{v}-\mathbf{U})^2 f_i(\mathbf{r},\mathbf{v},t)$$

Boltzmann collision operators $J_{ij}[f_i,f_j]$ *conserve* the particle number of each species and the total momentum

$$\int d\mathbf{v} J_{ij}[\mathbf{v}|f_i,f_j]=0, \qquad \sum_{i=1}^{2}\sum_{j=1}^{2}\int d\mathbf{v} m_i \mathbf{v} J_{ij}[\mathbf{v}|f_i,f_j]=0$$

but the total energy is ***not*** conserved

$$\sum_{i=1}^{2}\sum_{j=1}^{2} m_i \int d\mathbf{v} V^2 J_{ij}[\mathbf{v}|f_i,f_j]=-dnT\zeta \qquad \mathbf{V}=\mathbf{v}-\mathbf{U}$$

ζ : fractional energy changes per unit time (**cooling rate**)

Macroscopic balance equations

Balance equation for the *partial densities*

$$D_t n_i + n_i \nabla \cdot \mathbf{U} + m_i^{-1} \nabla \cdot \mathbf{j}_i = 0$$

Balance equation for the mean *flow velocity*

$$\rho D_t \mathbf{U} + \nabla \mathsf{P} = 0$$

Balance equation for the granular *temperature*

$$\frac{d}{2} n \left(D_t + \zeta \right) T + \mathsf{P} : \nabla \mathbf{U} + \nabla \cdot \mathbf{q} - \frac{d}{2} T \sum_{i=1}^{2} m_i^{-1} \nabla \cdot \mathbf{j}_i = 0$$

$$D_t = \partial_t + \mathbf{U} \cdot \nabla$$

Mass flux

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

Pressure or stress tensor

$$\mathsf{P} = \sum_{i=1}^{2} m_i \int d\mathbf{v}\, \mathbf{V}\mathbf{V}\, f_i(\mathbf{v})$$

Heat flux

$$\mathbf{q} = \sum_{i=1}^{2} \frac{m_i}{2} \int d\mathbf{v}\, V^2 \mathbf{V}\, f_i(\mathbf{v})$$

HOMOGENEOUS COOLING STATE

Spatially *homogeneous* isotropic states

$$\partial_t f_i(v,t) = \sum_j J_{ij}[v|f_i(t), f_j(t)]$$

Partial temperatures $\longrightarrow$ $n_i T_i = \frac{m_i}{d}\int d\mathbf{v}\, v^2 f_i(\mathbf{v})$

Granular temperature $\longrightarrow$ $T = \sum_i x_i T_i, \quad x_i = n_i/n$

Cooling rates for T_i $\longrightarrow$ $\zeta_i = -\partial_t \ln T_i, \quad \zeta = T^{-1}\sum_i x_i T_i \zeta_i$

$\zeta = -\partial_t \ln T$ $\longrightarrow$ $T(t) \propto t^{-2}$ Haff's law (1983)

$$\zeta_1 = \zeta_{11} + \zeta_{12}$$

$$\zeta_{11} = -\frac{m_1}{d n_1 T_1} \int d\mathbf{v} v^2 J_{11}[f_1, f_1]$$

→ Zero for *elastic* systems

$$\zeta_{12} = -\frac{m_1}{d n_1 T_1} \int d\mathbf{v} v^2 J_{12}[f_1, f_2]$$

→ *Nonzero* in general for *elastic* systems

If f_i are *Maxwellians* at the same temperature, then $\boldsymbol{\zeta_{12}=0}$ (elastic case). Detailed balance whereby the energy transfer between species is balanced by energy conservation for this state

The *analog* of the balance detailed state for *inelastic* systems:

Homogeneous cooling state (HCS)

Assumption

Hydrodynamic or ***normal*** state: all the *time* dependence of vdf occurs only through the temperature T(t)

$$f_i(v,t) = n_i v_0^{-d}(t)\Phi_i(v/v_0(t))$$

$$v_0^2(t) \propto T(t)$$

Consequence: ***temperature ratio*** $\gamma=T_1/T_2$ must be ***constant*** (independent of time)

HCS condition: $\partial_t \ln \gamma = \zeta_2 - \zeta_1 \longrightarrow \boxed{\zeta_1 = \zeta_2}$

Elastic collisions: $\zeta_1 = \zeta_2 = 0, \quad T_1 = T_2 = T$

$\downarrow$

Equipartition theorem for classical statistical mechanics

What happens if the collisions are **inelastic** ?

Well-posed *mathematical* problem: one has to solve the BE for the reduced distributions subject to $\zeta_1=\zeta_2$

So far, an ***exact*** solution is not known….

Approximate solution

$$\Phi_i(V^*) \to \left(\frac{\theta_i}{\pi}\right)^{d/2} e^{-\theta_i v^{*2}} \left[1+\frac{c_i}{4}\left(\theta_i^2 v^{*4}-(d+2)v^{*2}+\frac{d(d+2)}{4}\right)\right]$$

$$v^* = v/v_0, \quad \theta_i = \frac{m_j}{m_i+m_j}\frac{T}{T_i}, \quad i\neq j$$

Garzó&Dufty PRE **60**, 5706 (1999)

Time evolution of temperature ratio γ. Comparison with Monte Carlo simulations

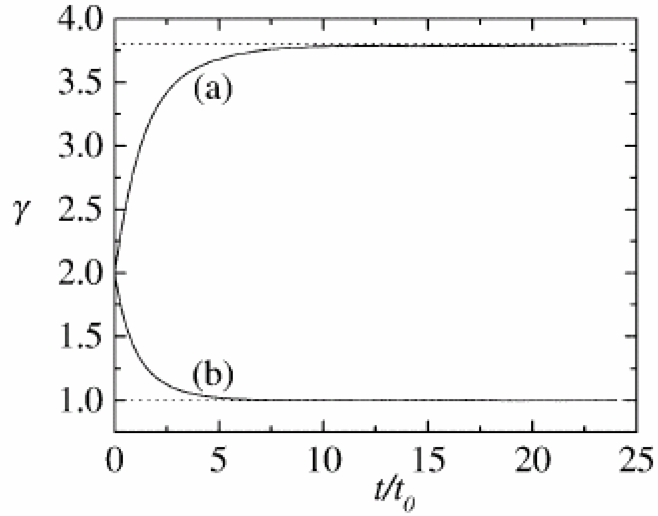


Fig. 1. Time evolution of $\gamma(t) = T_1(t)/T_2(t)$ for $n^* = 0$, $\delta = 2$, $w = 1$, $\mu = 10$, and $\alpha = 0.5$ (a) and $\alpha = 1$ (b). The dotted lines refer to the theoretical predictions. Time is measured in units of $t_0 \equiv \lambda_{11}/v_{01}(0)$

Montanero& Garzó, Gran Matt. **4**, 17 (2002)

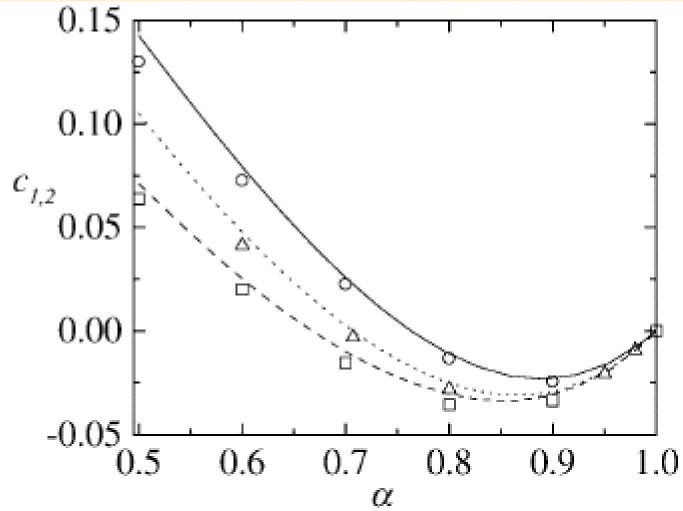


Fig. 2. Plot of the coefficients c_i versus the restitution coefficient α for $n^* = 0$, $\delta = 1$, $w = 1$ and $\mu = 2$. The solid line and the circles refer to c_1 while the dashed line and the squares correspond to c_2. The dotted line and the triangles refer to the common value in the single component case. The lines are the theoretical predictions and the symbols correspond to the simulation results

Garzó&Dufty PRE **60**, 5706 (1999)

Montanero& Garzó, Gran Matt. **4**, 17 (2002)

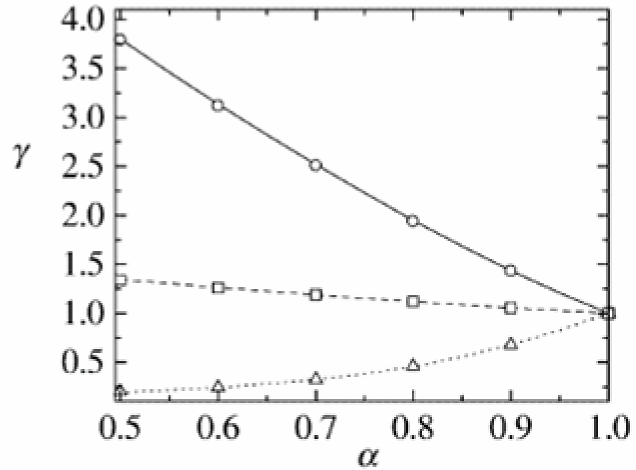


Fig. 4. Plot of the temperature ratio γ versus the restitution coefficient α for $n^* = 0$, $\delta = 2$, $w = 1$ and three different values of the mass ratio: $\mu = 1/10$ (dotted line and triangles), $\mu = 2$ (dashed line and squares) and $\mu = 10$ (solid line and circles). The lines are the theoretical predictions and the symbols correspond to the simulation results

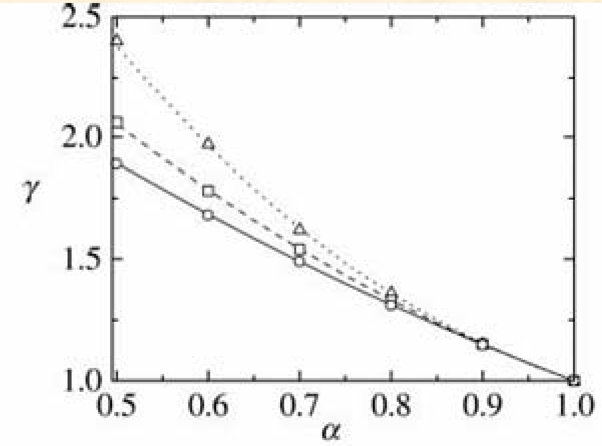


Fig. 5. Plot of the temperature ratio versus the restitution coefficient α for $n^* = 0$, $w = 1$, $\mu = 4$ and three different values of the concentration ratio: $\delta = 1/4$ (dotted line and triangles), $\delta = 1$ (dashed line and squares) and $\delta = 4$ (solid line and circles). The lines are the theoretical predictions and the symbols correspond to the simulation results

Comparison with *molecular dynamics* (MD) simulations

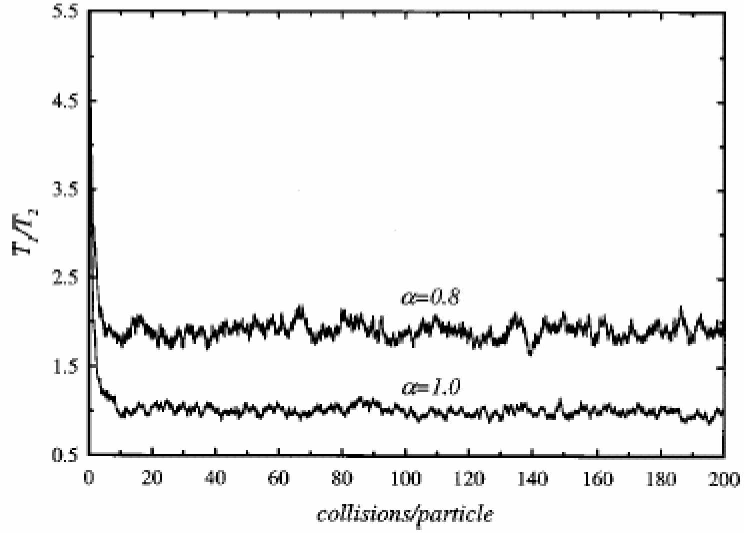


FIG. 1. Time evolution of $\gamma(t)=T_1(t)/T_2(t)$ for $\phi=0.1$, $\sigma_1/\sigma_2=\phi_1/\phi_2=1$, $m_1/m_2=8$, and two values of α: $\alpha=0.8$ and $\alpha=1$.

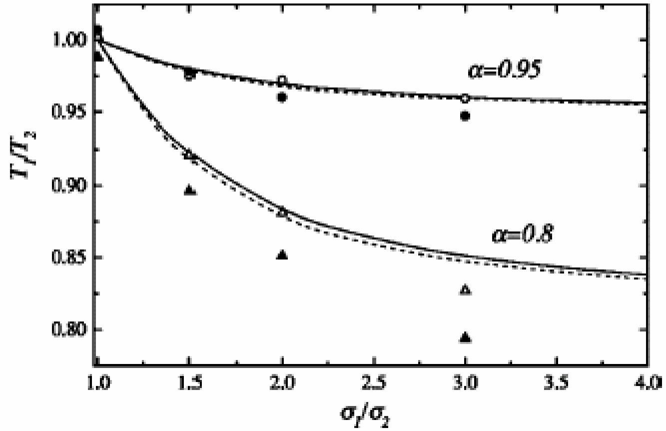


FIG. 3. Plot of the temperature ratio T_1/T_2 as a function of the size ratio σ_1/σ_2 for $m_1/m_2=\phi_1/\phi_2=1$, and two different values of α: $\alpha=0.95$ (lines and circles) and $\alpha=0.8$ (lines and triangles). The lines are the Enskog predictions and the symbols refer to the MD simulation results. The solid (dashed) lines correspond to $\phi=0.1$ ($\phi=0.2$), while the open (solid) symbols correspond to $\phi=0.1$ ($\phi=0.2$).

Dahl, Hrenya, Garzó& Dufty, PRE **66**, 041301 (2002)

Breakdown of energy equipartition

Computer simulation studies: Barrat&Trizac GM **4**, 57 (2002); Krouskop&Talbot, PRE **68**, 021304 (2003); Wang *et al*. PRE **68**, 031301 (2003); Brey et al. PRE **73**, 031301 (2006); Schroter *et al*. PRE **74**, 011307 (2006);…….

Real experiments: Wildman&Parker, PRL **88**, 064301 (2002); Feitosa&Menon, PRL **88**, 198301 (2002).

All these results ***confirm*** this new feature in granular mixtures !!

What is the **influence** of energy nonequipartition on ***transport properties*** of the granular mixture?

In particular, the mass flux is given by

$$\mathbf{j}_1 = -\frac{m_1 m_2 n}{\rho} D \nabla x_1 - \frac{\rho}{p} D_p \nabla p - \frac{\rho}{T} D_T \nabla T$$

Transport coefficients

For instance,

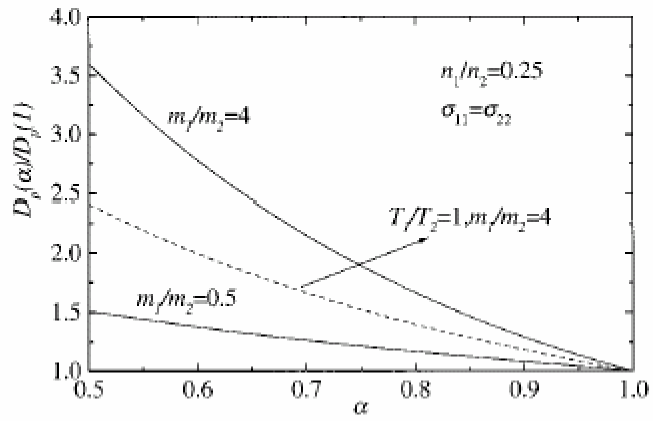
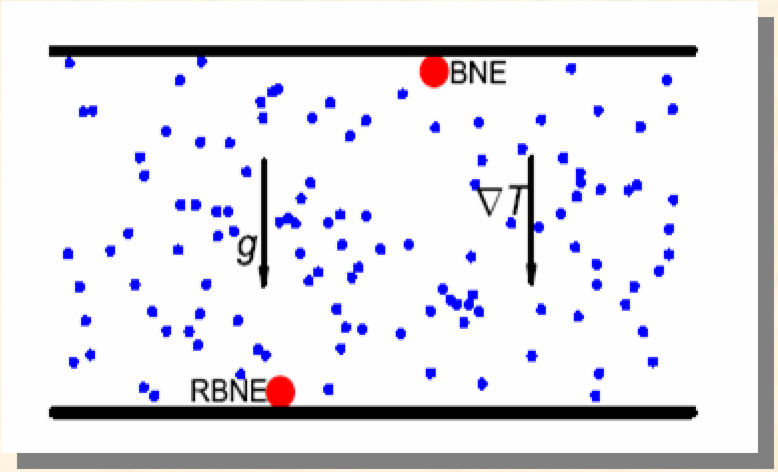


FIG. 1. Plot of the reduced pressure diffusion coefficient $D_p(\alpha)/D_p(1)$ as a function of the restitution coefficient $\alpha=\alpha_{11}=\alpha_{22}=\alpha_{12}$ for $\sigma_{11}=\sigma_{22}=\sigma_{12}$, a concentration ratio $n_1/n_2=0.25$, and two different values of the mass ratio: $m_1/m_2=0.5$ and $m_1/m_2=4$. The dashed line refers to the case $m_1/m_2=4$ by assuming the equality of the partial temperatures $\gamma=T_1/T_2=1$.

Garzó&Dufty, Phys. Fluids **14**, 1476 (2002)

Segregation of an intruder in a granular gas



Segregation driven by *gravity* and *thermal gradients*: thermal (Soret) diffusion

Order parameter for the transition BNE/RBNE

$$\theta = \frac{mT_0}{m_0 T}$$

Brey, Ruiz-Montero& Moreno PRL **95**, 098001 (2005); Garzó EPL **75**, 521 (2006)

If $\theta > 1$ ($\theta < 1$), then BNE (RBNE)

Due to the lack of energy equipartition, criterion is rather complicated since it involves all the parameter space

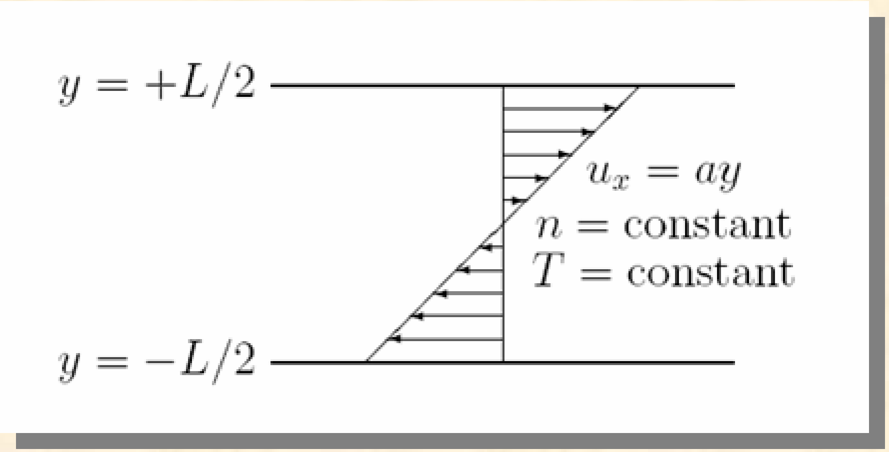
If $T_0 = T$, segregation is predicted for particles that differ only in mass !!

Consistent with experiments and simulations

SHEARED GRANULAR MIXTURES

Due to the kinetic energy dissipation in collisions, energy must be **externally** injected to fluidize the system and achieve stationary conditions.

Mechanism of energy input: Simple or **uniform shear flow** (USF)



Time evolution of the *granular temperature* arises from the balance of two opposite effects: viscous heating and collisional cooling. When the shearing work is balanced by the dissipation in collisions, a *steady* state is reached.

Steady state condition → $$aP_{xy} = -\frac{d}{2} nT\zeta$$

Intrinsic connection between the velocity gradient (*nonequilibrium* parameter) and dissipation (*coefficients of restitution*). Both parameters are **not** independent.

$$a^*(\alpha_{ij}) = \frac{a}{\nu(T)}, \qquad \nu(T) \propto \sqrt{T}$$

USF becomes spatially uniform in the local Lagrangian frame moving with the flow velocity ***U***

$$f_i(\mathbf{r},\mathbf{v}) \to f_i(\mathbf{V}), \qquad V_k = v_k - a_{k\ell} r_\ell$$

$$a_{k\ell} = a\delta_{kx}\delta_{\ell y}$$

Steady Boltzmann equation

$$-aV_y \frac{\partial}{\partial V_x} f_i = \sum_j J_{ij}[f_i, f_j]$$

Grad's approach

$$f_i \to f_{i,M}\left[1 + \frac{m_i}{2T_i}\left(\frac{P_{i,k\ell}}{n_i T_i} - \delta_{k,\ell}\right) V_k V_\ell\right]$$

$$P_{i,k\ell} = \int d\mathbf{V}\, m_i V_k V_\ell f_i$$

Partial temperatures

$$T_i = \frac{1}{dn_i} P_{i,kk}$$

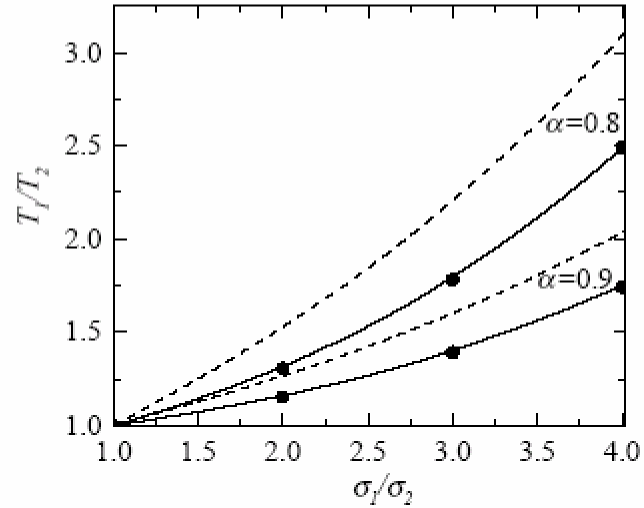
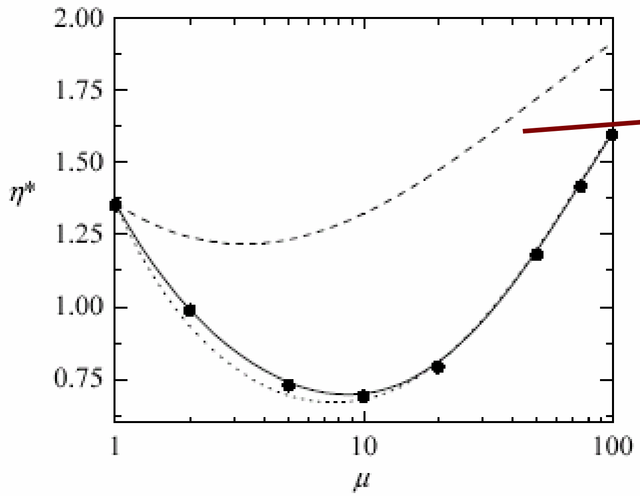


Fig. 11. Plot of the temperature ratio T_1/T_2 as a function of the size ratio $\sigma_1/\sigma_2 = (m_1/m_2)^{1/2}$ for a two-dimensional system in the case $x_1 = 1/2$ and two different values of the (common) coefficient of restitution: $\alpha = 0.9$ and $\alpha = 0.8$. The solid lines are the theoretical predictions based on Grad's solution, while the symbols refer to the DSMC results. The dashed lines correspond to the results obtained from the stochastic thermostat condition (31).

Montanero&Garzó, Physica A **310**, 17 (2002); Garzó PRE **66**, 021308 (2002)

Rheological properties $\eta^* = \dfrac{|P_{xy}|}{\rho_1 v_0 a^2}$

Garzó&Montanero, Gran. Matt. **5**, 165 (2003)



$T_1 = T_2$

Fig. 13. Plot of the reduced shear viscosity η^* versus the mass ratio $\mu = m_1/m_2$ for a two-dimensional system with $\sigma_1 = \sigma_2$, $x_1 = 1/2$ and $\alpha = 0.9$. The solid line corresponds to the theoretical predictions derived from Grad's solution, the dotted line refers to the latter theory but using the expression of T_1/T_2 obtained from the stochastic thermostat condition (31), and the dashed line is the result obtained from Grad's solution by assuming the equality of the partial temperatures ($\gamma = 1$). The symbols are the DSMC results.

CONCLUSIONS

✓Hydrodynamic description (derived from kinetic theory) appears to be a powerful tool for analysis and predictions of rapid flow gas dynamics of granular mixtures.

✓New and interesting result: partial temperatures (which measure the mean kinetic energy of each species) are different (breakdown of energy equipartition theorem). Not surprising feature since granular matter is inherently in non-equilibrium.

✓Energy nonequipartition has important and new quantitiative effects on macroscopic properties (transport coefficients, segregation criterion,…) of the system

Thanks for your attention and….

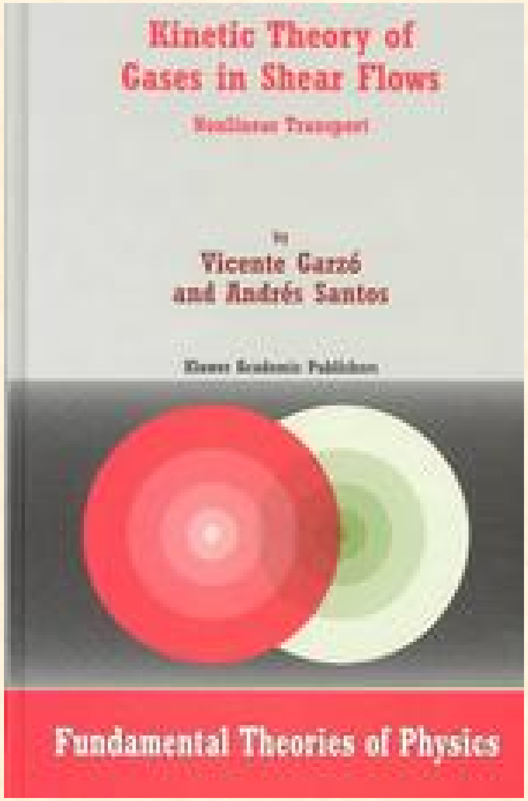
MOLTES FELICITATS, PEPE

Maxwell potential: nice mathematical properties of the Boltzmann collision operator

Velocity moment of order *k* of the Boltzmann collision operator

only involves moments of order less than or equal to *k*

Elastic fluids: Nonlinear transport properties



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