DENSE FLUID TRANSPORT FOR GRANULAR MIXTURES OF INELASTIC HARD SPHERES

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OUTLINE

- Motivation
- Enskog kinetic theory for granular mixtures
- Macroscopic balance equations
- Chapman-Enskog solution: Navier-Stokes transport coefficients
- Shear viscosity
- Tracer diffusion coefficients
- Conclusions

THE MOTIVATION

Granular media under rapid flow conditions: hydrodynamic-like type equations

Boltzmann and Enskog kinetic theories for *inelastic* disks or hard spheres. Chapman-Enskog method: *normal* solution as a perturbation expansion in the hydrodynamic gradients

Monocomponent granular gases: Brey et al. PRE (1998); Garzó&Dufty PRE (1999); Lutsko PRE (2005)

Real granular systems characterized by some degrees of polidispersity in density and size: ***Multicomponent*** granular systems

Some **previous** studies: Jenkins&Mancini, J. Appl. Mech. (1987); PF (1989); Zamankhan, PRE (1995); Arnarson&Willits PF (1998), (1999); Serero et al. JFM (2006)

Limited to the quasi-elastic limit ($\alpha_{ij} \approx 1$). Reference state: Maxwellians at the same temperature. However, many recent results (theory, simulations, experiments) have shown the *breakdown* of energy equipartition

Objective: Kinetic theory for multicomponent systems which incorporates nonequipartition effects, without restriction on α_{ij} and applicable for moderately dense flows

Low-density limit: Garzó&Dufty PF, **14** 1476 (2002)

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REVISED ENSKOG KINETIC THEORY

S-multicomponent mixture of smooth hard spheres or disks of masses m_i, diameters σ_i, and coefficients of restitution α_{ij}

At a kinetic level: $f_i(\mathbf{r}_1,\mathbf{v}_1;t)$

$$\left(\partial_t + \mathbf{v}_1 \cdot \nabla_{\mathbf{r}_1} + m_i^{-1}\mathbf{F}_i(\mathbf{r}_1) \cdot \nabla_{\mathbf{v}_1}\right) f_i(\mathbf{r}_1, \mathbf{v}_1; t) = C_i(\mathbf{r}_1, \mathbf{v}_1; t)$$

$$C_i(\mathbf{r}_1, \mathbf{v}_1; t) = \sum_{j=1}^{s} \sigma_{ij}^{d-1} \int d\mathbf{v}_2 \int d\widehat{\boldsymbol{\sigma}} \Theta(\widehat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12})(\widehat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12}) \times \left(\alpha_{ij}^{-2} f_{ij}(\mathbf{r}_1, \mathbf{v}_1'', \mathbf{r}_1 - \boldsymbol{\sigma}_{ij}, \mathbf{v}_2''; t) - f_{ij}(\mathbf{r}_1, \mathbf{v}_1, \mathbf{r}_1 + \boldsymbol{\sigma}_{ij}, \mathbf{v}_2; t)\right)$$

Two-particle distribution function

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Collision rules:

$$\mathbf{v}_1'' = \mathbf{v}_1 - \mu_{ji}\left(1+\alpha_{ij}^{-1}\right)(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})\widehat{\boldsymbol{\sigma}}$$

$$\mathbf{v}_2'' = \mathbf{v}_2 + \mu_{ij}\left(1+\alpha_{ij}^{-1}\right)(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})\widehat{\boldsymbol{\sigma}}$$

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

Kinetic theory approach: ***velocity*** correlations are neglected

$$f_{ij}(\mathbf{r}_1,\mathbf{v}_1,\mathbf{r}_2,\mathbf{v}_2;t) \to \chi_{ij}\left(\mathbf{r}_1,\mathbf{r}_2 \mid \{n_i\}\right) f_i(\mathbf{r}_1,\mathbf{v}_1;t) f_j(\mathbf{r}_2,\mathbf{v}_2;t)$$

Spatial correlations (volume exclusion effects)

Uniform systems:

$$g_{ij}\left(\sigma_{ij};\{n_k\}\right) = \frac{1+\alpha_{ij}}{2\alpha_{ij}}\chi_{ij}\left(\sigma_{ij};\{n_k\}\right)$$

Pair correlation function

J. Lutsko, PRE 63, 061211 (2001)

Bad news for the RET: Several MD simulations have shown that velocity correlations become *important* as density increases (McNamara&Luding, PRE (1998); Soto&Mareschal PRE (2001); Pagonabarraga et al. PRE (2002))

Good news for the RET: Good agreement at the level of *macroscopic* properties for moderate densities and finite dissipation (Simulations: Brey et al., PF (2000) ; Lutsko, PRE (2001); Dahl et al., PRE (2002)
Experiments: Yang et al., PRL (2002); PRE (2004))

We (Christine, Jim and myself) think that the RET is *still* a valuable theory for granular fluids for *densities* beyond the Boltzmann limit and *dissipation* beyond the quasielastic limit.

MACROSCOPIC BALANCE EQUATIONS

Hydrodynamic fields

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

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

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

Enskog collision operators $J_{ij}[f_i,f_j]$ *conserve* the particle number of each species and the total momentum, but the total energy is ***not*** conserved (cooling rate ζ)

Macroscopic equations are ***exact*** since they are obtained from the first hierarchy equation (without the Enskog approximation)

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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 flow velocity

$$\rho D_t U_\beta + \partial_{r_\gamma} P_{\gamma\beta} = \sum_{i=1}^{s} n_i(\mathbf{r}, t) F_{i\beta}(\mathbf{r})$$

Balance equation for the granular temperature

$$\frac{d}{2} n (D_t + \zeta) T + P_{\gamma\beta} \partial_{r_\gamma} U_\beta + \nabla \cdot \mathbf{q} - \frac{d}{2} T \sum_{i=1}^{s} m_i^{-1} \nabla \cdot \mathbf{j}_i = \sum_{i=1}^{s} m_i^{-1} \mathbf{F}_i \cdot \mathbf{j}_i$$

$$D_t \equiv \partial_t + \mathbf{v} \cdot \nabla$$

Mass flux $\mathbf{j}_i(\mathbf{r}_1,t) = m_i \int d\mathbf{v}_1 \mathbf{V}_1 f_i(\mathbf{r}_1,\mathbf{v}_1;t)$

V=v-U

Pressure tensor $P_{\gamma\beta}(\mathbf{r}_1,t) = P^k_{\gamma\beta}(\mathbf{r}_1,t) + P^c_{\gamma\beta}(\mathbf{r}_1,t)$

Kinetic contribution **Collisional contribution**

$$P^k_{\gamma\beta}(\mathbf{r}_1,t) = \sum_{i=1}^{s} \int d\mathbf{v}_1 m_i V_{1\beta} V_{1\gamma} f_i(\mathbf{r}_1,\mathbf{v}_1;t)$$

$$P^c_{\gamma\beta}(\mathbf{r}_1,t) = \frac{1}{2}\sum_{i,j=1}^{s} m_j \mu_{ij}\left(1+\alpha_{ij}\right)\sigma^d_{ij} \int d\mathbf{v}_1 \int d\mathbf{v}_2 \int d\widehat{\boldsymbol{\sigma}}\, \Theta(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})^2 \times \widehat{\sigma}_\beta \widehat{\sigma}_\gamma \int_0^1 dx\, f_{ij}(\mathbf{r}_1 - x\boldsymbol{\sigma}_{ij}, \mathbf{v}_1, \mathbf{r}_1 + (1-x)\boldsymbol{\sigma}_{ij}, \mathbf{v}_2; t).$$

Heat flux $\mathbf{q}(\mathbf{r}_1,t)=\mathbf{q}^k(\mathbf{r}_1,t)+\mathbf{q}^c(\mathbf{r}_1,t)$

$$\mathbf{q}^k(\mathbf{r}_1,t)=\sum_{i=1}^{s}\int d\mathbf{v}_1\frac{1}{2}m_iV_1^2\mathbf{V}_1f_i(\mathbf{r}_1,\mathbf{v}_1;t)$$

$$\begin{aligned}\mathbf{q}^c(\mathbf{r}_1,t) &= \sum_{i,j=1}^{s}\frac{1}{8}\left(1+\alpha_{ij}\right)m_j\mu_{ij}\sigma_{ij}^d\int d\mathbf{v}_1\int d\mathbf{v}_2\int d\widehat{\boldsymbol{\sigma}}\,\Theta(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})\\ &\times(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})^2\left[\left(1-\alpha_{ij}\right)\left(\mu_{ji}-\mu_{ij}\right)(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})+4\widehat{\boldsymbol{\sigma}}\cdot\mathbf{G}_{ij}\right)\\ &\times\widehat{\boldsymbol{\sigma}}\int_0^1 dx\,f_{ij}(\mathbf{r}_1-x\boldsymbol{\sigma}_{ij},\mathbf{v}_1,\mathbf{r}_1+(1-x)\,\boldsymbol{\sigma}_{ij},\mathbf{v}_2;t),\end{aligned}$$

$\mathbf{G}_{ij}=\mu_{ij}\mathbf{V}_1+\mu_{ji}\mathbf{V}_2$ is the center-of-mass velocity

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Cooling rate

$$\zeta = \frac{1}{2dnT}\sum_{i,j=1}^{s}\left(1-\alpha_{ij}^{2}\right) m_i \mu_{ji} \sigma_{ij}^{d-1} \int d\mathbf{v}_1 \int d\mathbf{v}_2 \int d\widehat{\boldsymbol{\sigma}} \times \Theta(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})^3 f_{ij}(\mathbf{r}_1,\mathbf{v}_1,\mathbf{r}_1+\boldsymbol{\sigma}_{ij},\mathbf{v}_2;t)$$

Balance equations become a closed set of hydrodynamic equations for (n_i,**U**,T) once the *fluxes* and the *cooling rate* are expressed as ***functionals*** of (n_i,**U**,T) ("constitutive relations")

Derivation of hydrodynamics ⟶ ***Normal*** solution to the RET

CHAPMAN-ENSKOG NORMAL SOLUTION

Assumption: For long times (much longer than the mean free time) and far away from boundaries (bulk region) the system reaches a *hydrodynamic* regime.

Normal solution $$f_i(\mathbf{r},\mathbf{v};t) = f_i(\mathbf{v}|\{n_i(\mathbf{r},t)\},\mathbf{U}(\mathbf{r},t),T(\mathbf{r},t)\})$$

This representation can also apply for situations where spatial gradients are ***not*** small so that f_i may be a nolinear function of the gradients (simple shear flow, for instance). In some situations, gradients are controlled by boundary or initial conditions:

$$f_i = f_i^{(0)} + \epsilon f_i^{(1)} + \cdots$$

LOCAL HOMOGENEOUS COOLING STATE

Since T(t), the reference state $f_i^{(0)}$ is not the local equilibrium distribution. Its explicit form is not known

$$-\zeta^{(0)} T \partial_T f_i^{(0)} = \sum_{j=1}^{s} J_{ij}^{(0)}[f_i^{(0)}, f_j^{(0)}]$$

Scaled form: $$f_i^{(0)}(V,t) = n_i v_o^{-d}(T(t)) \Phi_i(V/v_o(T(t)))$$

Sonine polynomial expansion

Normal solution → Temperature ratios must be independent of time

$$\zeta_1^{(0)} = \zeta_2^{(0)} = \cdots = \zeta_s^{(0)}$$

$$\partial_t T_i^{(0)} = -\zeta_i^{(0)} T_i^{(0)}, \quad d n_i T_i^{(0)} = \int d\mathbf{v} m_i V^2 f_i^{(0)}$$

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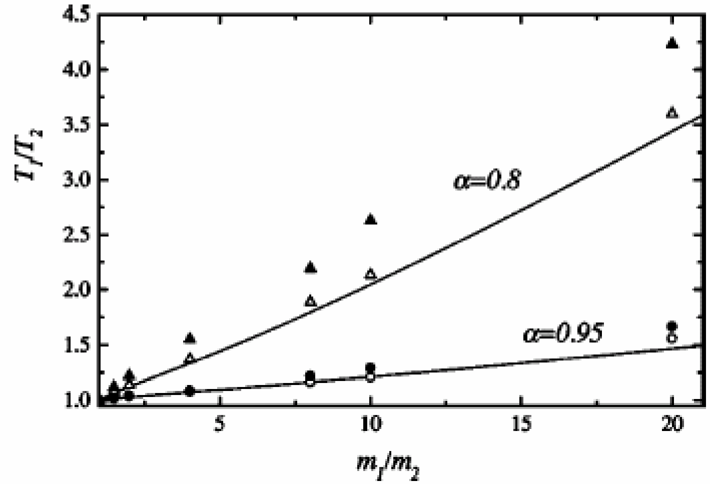

FIG. 2. Plot of the temperature ratio T_1/T_2 as a function of the mass ratio m_1/m_2 for $\sigma_1/\sigma_2=\phi_1/\phi_2=1$, and two different values of α: $\alpha=0.95$ (solid line and circles) and $\alpha=0.8$ (solid line and triangles). The lines are the Enskog predictions and the symbols refer to the MD simulation results. The open (solid) symbols correspond to $\phi=0.1$ ($\phi=0.2$).

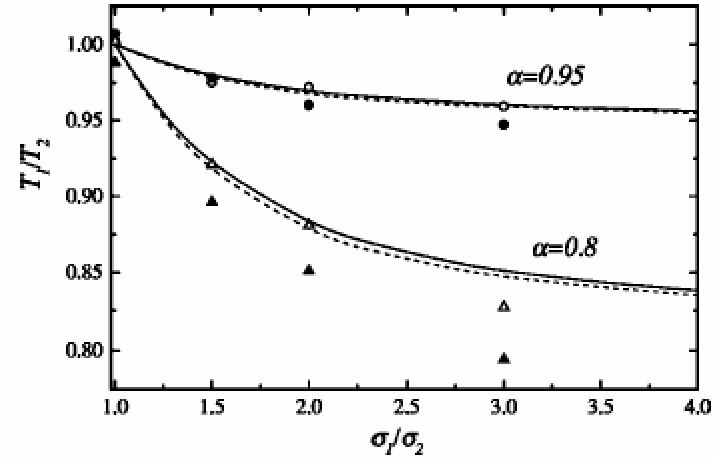

FIG. 3. Plot of the temperature ratio T_1/T_2 as a function of the size ratio σ_1/σ_2 for $m_1/m_2=\phi_1/\phi_2=1$, and two different values of α: $\alpha=0.95$ (lines and circles) and $\alpha=0.8$ (lines and triangles). The lines are the Enskog predictions and the symbols refer to the MD simulation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

Garzó&Dufty, PRE **60**, 5706 (1999)

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

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NAVIER-STOKES HYDRODYNAMIC EQUATIONS

Motivation: determine the transport coefficients *without* limitation to the degree of dissipation

The distribution functions are given by

$$
\begin{aligned}
f_i^{(1)}(\mathbf{V}) \;=\; & \mathcal{A}_i(\mathbf{V}) \cdot \nabla \ln T + \sum_{j=1}^{s} \mathcal{B}_i^j(\mathbf{V}) \cdot \nabla \ln n_j \\
& + \mathcal{C}_{i,\gamma\eta}(\mathbf{V}) \frac{1}{2}\left(\partial_\gamma U_\eta + \partial_\eta U_\gamma - \frac{2}{d}\delta_{\gamma\eta} \nabla \cdot \mathbf{U} \right) \\
& + \mathcal{D}_i(\mathbf{V}) \nabla \cdot \mathbf{U} + \sum_{j=1}^{s} \mathcal{E}_i^j(\mathbf{V}) \cdot \mathbf{F}_j
\end{aligned}
$$

After some efforts….

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$$\left(\left(\mathcal{L}-\frac{1}{2}\zeta^{(0)}\right)\boldsymbol{\mathcal{A}}\right)_i=\mathbf{A}_i$$

$$\left(\mathcal{L}\boldsymbol{\mathcal{B}}^j\right)_i-n_j\frac{\partial\zeta^{(0)}}{\partial n_j}\boldsymbol{\mathcal{A}}_i=\mathbf{B}_i^j$$

$$\left(\left(\mathcal{L}+\frac{1}{2}\zeta^{(0)}\right)\mathcal{C}_{\gamma\eta}\right)_i=C_{i,\gamma\eta}$$

$$\left(\left(\mathcal{L}+\frac{1}{2}\zeta^{(0)}\right)\mathcal{D}\right)_i=D_i$$

$$\left(\left(\mathcal{L}+\zeta^{(0)}\right)\boldsymbol{\mathcal{E}}^j\right)_i=\mathbf{E}_i^j$$

Inhomogeneous terms are defined in terms of $f_i^{(0)}$

CONSTITUTIVE EQUATIONS

A. Cooling rate

$$\zeta \to \zeta^{(0)} + \zeta_U \nabla \cdot \mathbf{U}$$

$$\zeta^{(0)} = \frac{B_3}{2dnT} \sum_{i,j=1}^{s} \left(1-\alpha_{ij}^2\right) \frac{m_i m_j}{m_i+m_j} \chi_{ij}^{(0)} \sigma_{ij}^{d-1} \int d\mathbf{v}_1 \int d\mathbf{v}_2 f_i^{(0)}(V_1) f_j^{(0)}(V_2)\, g_{12}^3$$

$$\zeta_U = -\frac{d+2}{dnT} B_4 \sum_{i,j=1}^{s} \left(1-\alpha_{ij}^2\right) \mu_{ji} \chi_{ij}^{(0)} \sigma_{ij}^{d} n_i n_j T_i^{(0)} + \frac{B_3}{dnT} \sum_{i,j=1}^{s} \left(1-\alpha_{ij}^2\right) \frac{m_i m_j}{m_i+m_j} \chi_{ij}^{(0)} \sigma_{ij}^{d-1} \int d\mathbf{v}_1 \int d\mathbf{v}_2\, g_{12}^3 f_i^{(0)}(\mathbf{V}_1) \mathcal{D}_j(\mathbf{V}_2)$$

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B. Mass fluxes

$$\mathbf{j}_i = -\sum_{j=1}^{s} m_i m_j \frac{n_j}{\rho} D_{ij} \nabla \ln n_j - \rho D_i^T \nabla \ln T - \sum_{j=1}^{s} D_{ij}^F \mathbf{F}_j$$

Transport coefficients :

$$D_i^T = -\frac{m_i}{\rho d} \int d\mathbf{v} \mathbf{V} \cdot \boldsymbol{\mathcal{A}}_i(\mathbf{V})$$

$$D_{ij} = -\frac{\rho}{m_j n_j d} \int d\mathbf{v} \mathbf{V} \cdot \boldsymbol{\mathcal{B}}_i^j(\mathbf{V})$$

$$D_{ij}^F = -\frac{m_i}{d} \int d\mathbf{v} \mathbf{V} \cdot \boldsymbol{\mathcal{E}}_i^j(\mathbf{V})$$

B. Pressure tensor

$$P_{\gamma\beta} = p\delta_{\gamma\beta} - \eta\left(\nabla_\gamma U_\beta + \nabla_\beta U_\gamma - \frac{2}{d}\nabla\cdot\mathbf{U}\right) - \kappa\nabla\cdot\mathbf{U}$$

Equation of state

$$p = nT + B_2 \sum_{i,j=1}^{s} \mu_{ji}\left(1+\alpha_{ij}\right)\sigma_{ij}^d \chi_{ij}^{(0)} n_i n_j T_i^{(0)}$$

Shear viscosity

$$\eta = \eta^k + \eta^c$$

$$\eta^k = \sum_{i=1}^{s} \eta_i^k = -\frac{1}{(d+2)(d-1)} \sum_{i=1}^{s} \int d\mathbf{v} m_i V_\lambda V_\gamma \mathcal{C}_{i,\lambda\gamma}(\mathbf{V})$$

$$\eta^c = \frac{2B_2}{(d+2)} \sum_{i,j=1}^{s} \mu_{ij}\left(1+\alpha_{ij}\right)\chi_{ij}^{(0)} n_i \sigma_{ij}^d \eta_j^k + \frac{d}{d+2}\kappa^c$$

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Bulk viscosity

$$\kappa = \kappa^k + \kappa^c$$

$$\kappa^k = 0$$

$$\kappa^c = \frac{B_3(d+1)}{2d^2} \sum_{i,j=1}^{s} m_j \mu_{ij} \left(1+\alpha_{ij}\right) \chi_{ij}^{(0)} \sigma_{ij}^{d+1} \times \int d\mathbf{v}_1 \int d\mathbf{v}_2 f_i^{(0)}(\mathbf{V}_1) f_j^{(0)}(\mathbf{V}_2) g_{12}$$

C. Energy flux

$$\mathbf{q} = -\lambda \nabla T - \sum_{i,j=1}^{s} \left(T^2 D_{q,ij} \nabla \ln n_j + L_{ij} \mathbf{F}_j \right)$$

Transport coefficients λ=λ^k+λ^c, …

$$\lambda^k = \sum_{i=1}^{s} \lambda_i^k = -\frac{1}{dT} \sum_{i=1}^{s} \int d\mathbf{v} \frac{1}{2} m_i V^2 \mathbf{V} \cdot \mathcal{A}_i (\mathbf{V})$$

$$D_{q,ij}^k = -\frac{1}{dT^2} \int d\mathbf{v} \frac{1}{2} m_i V^2 \mathbf{V} \cdot \mathcal{B}_i^j (\mathbf{V})$$

$$L_{ij}^k = -\frac{1}{d} \int d\mathbf{v} \frac{1}{2} m_i V^2 \mathbf{V} \cdot \mathcal{E}_i^j (\mathbf{V})$$

$$\lambda^c = \sum_{i,j=1}^{s} \frac{1}{8}\left(1+\alpha_{ij}\right) m_j \mu_{ij} \sigma_{ij}^d \chi_{ij}^{(0)} \left\{ 2B_4 \left(1-\alpha_{ij}\right)\left(\mu_{ij}-\mu_{ji}\right) n_i \left[\frac{2}{m_j}\lambda_j^k + (d+2)\frac{T_i^{(0)}}{m_i m_j T}\rho D_j^T\right] + \frac{8B_2}{2+d} n_i \left[\frac{2\mu_{ij}}{m_j}\lambda_j^k - (d+2)\frac{T_i^{(0)}}{m_i m_j T}\left(2\mu_{ij}-\mu_{ji}\right)\rho D_j^T\right] - T^{-1} C_{ij}^T \right\}$$

$$D_{q,ij}^c = \sum_{p=1}^{s} \frac{1}{8}\left(1+\alpha_{ip}\right) m_p \mu_{ip} \sigma_{ip}^d \chi_{ip}^{(0)} \left\{ 2B_4 \left(1-\alpha_{ip}\right)\left(\mu_{ip}-\mu_{pi}\right) \times n_i \left[\frac{2}{m_p} D_{q,pj}^k + (d+2)\frac{T_i^{(0)}}{T^2}\frac{m_j n_j}{\rho m_i} D_{pj}\right] + \frac{8B_2}{d+2} n_i \left[\frac{2\mu_{pi}}{m_p} D_{q,pj}^k - (d+2)\left(2\mu_{ip}-\mu_{pi}\right)\frac{T_i^{(0)}}{T^2}\frac{n_j m_j}{m_i \rho} D_{pj}\right] - T^{-2} C_{ipj}^T \right\}$$

$$L_{ij}^c = \sum_{p=1}^{s} \frac{1}{8}\left(1+\alpha_{ip}\right) m_p \mu_{ip} \sigma_{ip}^d \chi_{ip}^{(0)} \left\{ 2B_4 \left(1-\alpha_{ip}\right)\left(\mu_{ip}-\mu_{pi}\right) \times n_i \left[\frac{2}{m_p} L_{pj}^k + (d+2)\frac{T_i^{(0)}}{m_i m_p} D_{pj}^F\right] + \frac{8B_2}{d+2} n_i \left[\frac{2\mu_{pi}}{m_p} L_{pj}^k - (d+2)\left(2\mu_{ip}-\mu_{pi}\right)\frac{T_i^{(0)}}{m_i m_p} D_{pj}^F\right] \right\}$$

Some *limiting* cases

- ✓ Mechanically equivalent particles [Garzó&Dufty PRE **59**, 5895 (1999)+Lutsko, PRE **72** 021306 (2005)]

- ✓ Binary mixtures at low-density [Garzó&Dufty, PF **14**, 1476 (2002)+Garzó&Montanero, JSP **129**, 27(2007)]

- ✓ Elastic hard spheres [López de Haro, Cohen&Kincaid, JCP **78**, 2746 (1983)]

Self-consistency of our results

Cooling rate and Navier-Stokes transport coefficients

$$\{\zeta^{(0)}, \zeta_U, D_{ij}, D_{ij}^T, D_{ij}^F, \eta, \kappa, \lambda, D_{q,ij}, L_{ij}\}$$

Coefficients are given in terms of $f_i^{(0)}$ and $f_i^{(1)}$: *Approximate* methods (Sonine polynomial expansion)

In some cases, $f_i^{(0)}(\mathbf{V}) \to f_{i,M}(\mathbf{V}) = n_i \left(\frac{m_i}{2\pi T_i}\right)^{d/2} \exp\left(-\frac{m_i V^2}{2T_i}\right)$

Generalized Carnahan-Starling form (d=3)

$$\chi_{ij}^{(0)} = \frac{1}{1-\phi} + \frac{10-\phi}{16} \frac{\beta}{(1-\phi)^2} \frac{\sigma_i \sigma_j}{\sigma_{ij}} - \frac{1}{16} \frac{\beta^2}{\phi(1-\phi)} \left(\frac{\sigma_i \sigma_j}{\sigma_{ij}}\right)^2$$

Shear viscosity coefficient of a heated binary mixture

From a computational point of view, it is difficult to measure this coefficient. **Strategy**: (Driven) simple shear flow

n_i=const., $\nabla T=0$, $U_{i,x}=ay$

Ordinary fluid (elastic collisions): T(t) due to *viscous heating*.

Average collision frequency $\nu(t) \propto T(t)^{1/2}$ (hard spheres). Thus,

$a^*=a/\nu(t) \to 0$ and so, one can *measure* the N-S shear viscosity in the long time limit [Naitoh&Ono, JCP (1979); Montanero&Santos PRE (1996)]

$$\frac{\nu}{nT}\eta = -\lim_{t\to\infty}\frac{P^*_{xy}}{a^*}, \qquad P^*_{xy} = P_{xy}/nT$$

Granular fluid (inelastic collisions): Energy sink in the temperature balance equation

$$\partial_t T = -\frac{2}{dn} a P_{xy} + (-\zeta T)$$

Is is possible to ***frustrate*** the cooling effects so that the viscous heating is still able to heat the system as in the elastic case? One can identify the (heated) shear viscosity when $a^* \to 0$

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Granular fluid is excited by an external energy source that exactly compensates for the collisional cooling (Gaussian thermostat)

$$\mathbf{F}_i^{\text{exc}}(\mathbf{V}) = \frac{1}{2} m_i \zeta \mathbf{V}$$

Kinetic theory: First Sonine approximation to get η of a heated granular binary mixture:

$$\mathcal{C}_{i,\gamma\beta}(\mathbf{V}) \to -f_{i,M}(\mathbf{V}) \frac{\eta_i^k}{n_i T_i^2} m_i \left(V_\gamma V_\beta - \frac{1}{d} V^2 \delta_{\gamma\beta} \right)$$

The expression of η slightly differs from the one obtained in the free cooling case

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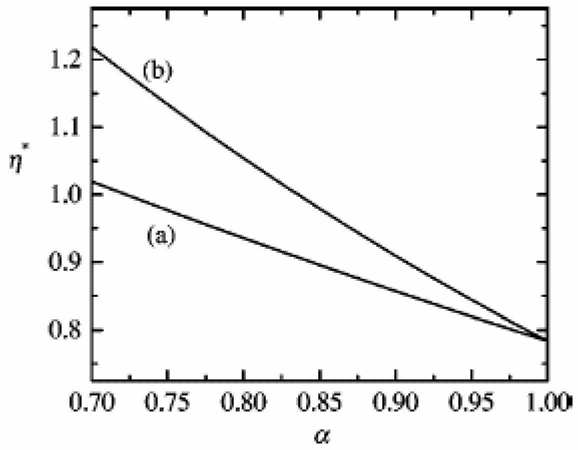

FIG. 1. Plot of the reduced shear viscosity η^* as a function of the restitution coefficient α for a binary mixture with parameters $\phi=0$, $x_1=1/2$, $\sigma_1/\sigma_2=1$, and $m_1/m_2=4$ in (a) the unforced case ($\xi^{(0)}=0$) and (b) the forced case ($\xi^{(0)}=\zeta^{(0)}$).

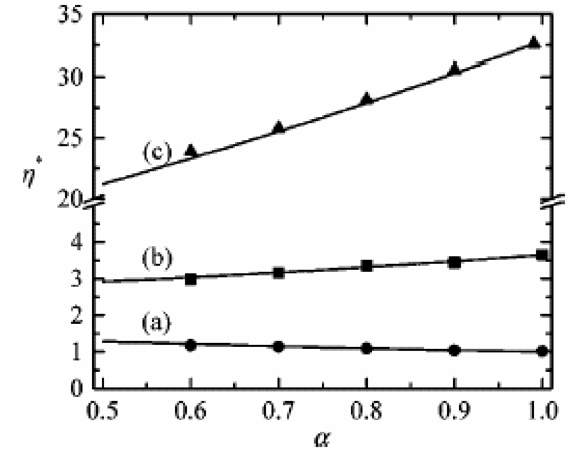

FIG. 3. Plot of the reduced shear viscosity η^* of a monocomponent gas as a function of the restitution coefficient α for three different values of the solid fraction ϕ: (a) $\phi=0$ (circles), (b) $\phi=0.2$ (squares), and (c) $\phi=0.4$ (triangles). The lines are the theoretical predictions and the symbols refer to the results obtained from Monte Carlo simulations.

Garzó&Montanero, PRE **68** 041302 (2003)

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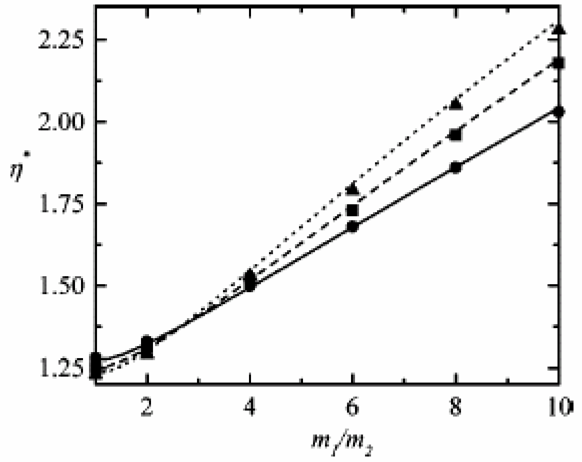


FIG. 6. Plot of the reduced shear viscosity η^* as a function of the mass ratio m_1/m_2, for $\phi=0.2$, $\sigma_1/\sigma_2=1$, $x_1=1/2$ and three different values of the restitution coefficient α: $\alpha=0.9$ (solid line and circles), $\alpha=0.8$ (dashed line and squares), and $\alpha=0.7$ (dotted line and triangles). The lines are the theoretical predictions and the symbols refer to the results obtained from Monte Carlo simulations.

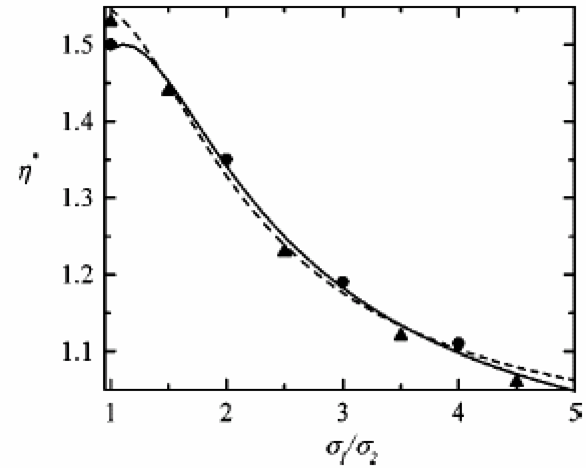


FIG. 7. Plot of the reduced shear viscosity η^* as a function of the size ratio σ_1/σ_2 for $\phi=0.2$, $m_1/m_2=4$, $x_1=1/2$ and two different values of the restitution coefficient α: $\alpha=0.9$ (solid line and circles) and $\alpha=0.7$ (dashed line and triangles). The lines are the theoretical predictions and the symbols refer to the results obtained from Monte Carlo simulations.

Mass transport of impurities

Tracer limit: $x_1 \rightarrow 0$. Diffusion of impurities in a dense granular gas. The state of the gas is not perturbed by impurities:

$$f_2^{(1)} = \mathcal{A}_2 \cdot \nabla T + \mathcal{C}_2 \cdot \nabla n_2$$

First-order distribution function of impurities

$$f_1^{(1)} = \mathcal{A}_1 \cdot \nabla T + \mathcal{B}_1 \cdot \nabla n_1 + \mathcal{C}_1 \cdot \nabla n_2 + \mathcal{E}_1 \cdot \mathbf{F}_1$$

Mass flux of impurities

$$\mathbf{j}_1^{(1)} = -\frac{m_1^2}{\rho} D_{11} \nabla n_1 - \frac{m_2 m_1}{\rho} D_{12} \nabla n_2 - \frac{\rho}{T} D_1^T \nabla T - D_{11}^F \mathbf{F}_1$$

$$D_1^T = -\frac{m_1}{\rho d} \int d\mathbf{v} \mathbf{V} \cdot \boldsymbol{\mathcal{A}}_1 (\mathbf{V})$$

$$D_{11} = -\frac{\rho}{m_1 n_1 d} \int d\mathbf{v} \mathbf{V} \cdot \boldsymbol{\mathcal{B}}_1 (\mathbf{V})$$

$$D_{12} = -\frac{1}{d} \int d\mathbf{v} \mathbf{V} \cdot \boldsymbol{\mathcal{C}}_1 (\mathbf{V})$$

$$D_{11}^F = -\frac{m_1}{d} \int d\mathbf{v} \mathbf{V} \cdot \boldsymbol{\mathcal{E}}_1 (\mathbf{V})$$

The corresponding integral equations verifying the unkowns are solved by considering the **two** first Sonine approximations

$$\boldsymbol{\mathcal{A}}_1(\mathbf{V}) \to -f_{1,M}(\mathbf{V}) \left[\frac{\rho}{n_1 T_1} \mathbf{V} D_1^T + a_1 \mathbf{S}_1(\mathbf{V}) \right]$$

$$\boldsymbol{\mathcal{B}}_1(\mathbf{V}) \to -f_{1,M}(\mathbf{V}) \left[\frac{m_1^2}{\rho T_1} \mathbf{V} D_{11} + b_1 \mathbf{S}_1(\mathbf{V}) \right]$$

$$\boldsymbol{\mathcal{C}}_1(\mathbf{V}) \to -f_{1,M}(\mathbf{V}) \left[\frac{m_1}{n_1 T_1} \mathbf{V} D_{12} + c_1 \mathbf{S}_1(\mathbf{V}) \right]$$

$$\boldsymbol{\mathcal{E}}_1(\mathbf{V}) \to -f_{1,M}(\mathbf{V}) \left[\frac{1}{n_1 T_1} \mathbf{V} D_{11}^F + e_1 \mathbf{S}_1(\mathbf{V}) \right]$$

$$\mathbf{S}_1(\mathbf{V}) = \left(\frac{1}{2} m_1 V^2 - \frac{d+2}{2} T_1 \right) \mathbf{V}$$

Parameter space: $\{m_1/m_2, \sigma_1/\sigma_2, \alpha_{12}, \alpha_{22}, \phi\}$

$$\phi \equiv \frac{\pi^{d/2}}{2^{d-1} d \Gamma(d/2)} n_2 \sigma_2^d$$

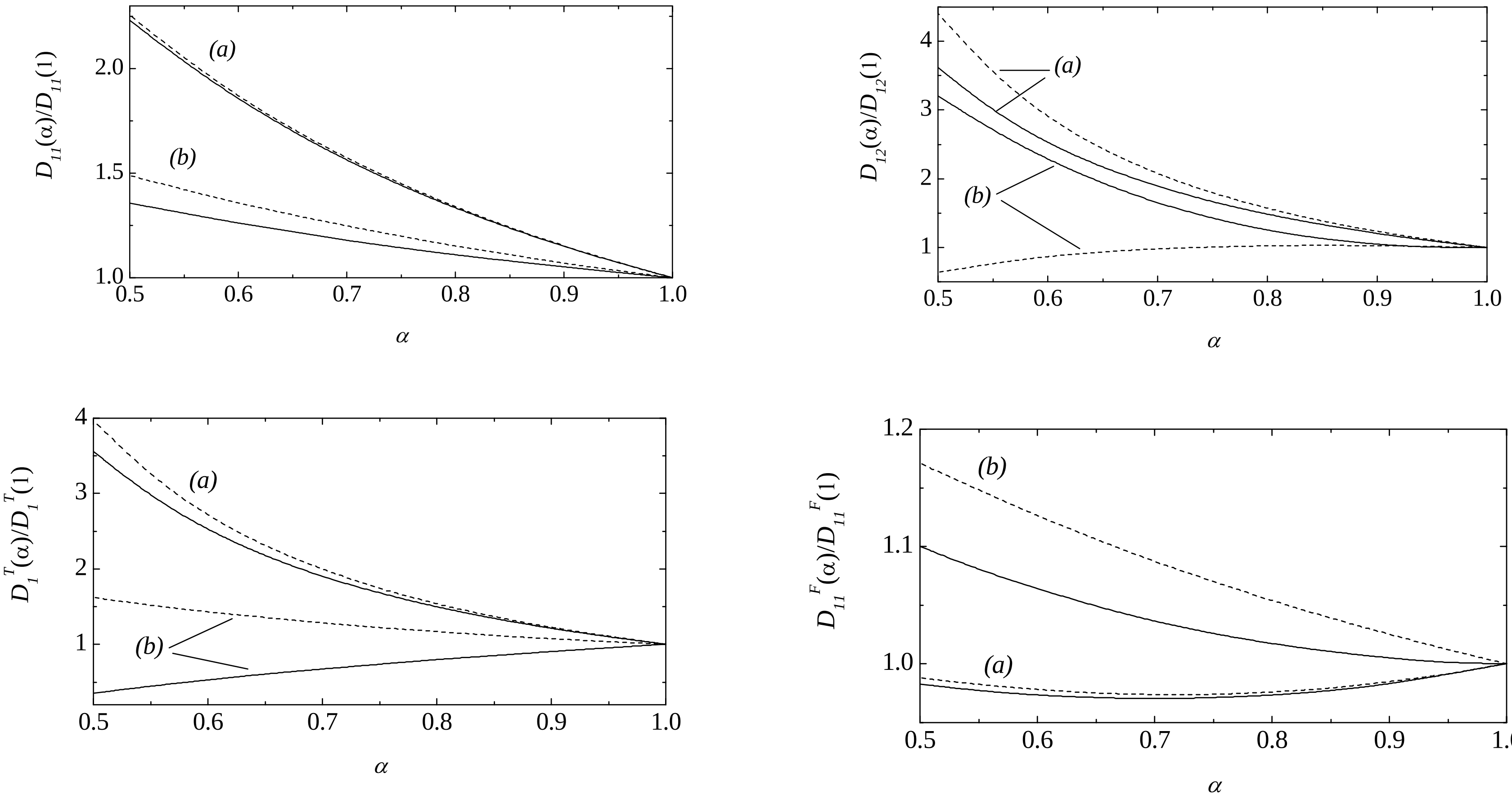
When the excess gas is in HCS, the diffusion equation is

$$\partial_t x_1(\mathbf{r}, t) = D_{11}(t)\nabla^2 x_1, \quad D_{11}(t) \propto \sqrt{T(t)}$$

Mean square position of impurity after a time interval t

$$\frac{\partial}{\partial t}\langle|\mathbf{r}(t) - \mathbf{r}(0)|^2\rangle = \frac{2dD_{11}(t)}{n_2}$$

Einstein form is used to measure D_{11} in DSMC simulations [Brey et al. PF **12**, 876 (2000)]



$(a) m_1/m_2 = 4; \sigma_1/\sigma_2 = 2, \quad (b) m_1/m_2 = 0.5; \sigma_1/\sigma_2 = 0.8$

$\alpha_{22} = \alpha_{12} \equiv \alpha, \quad \phi = 0.1$

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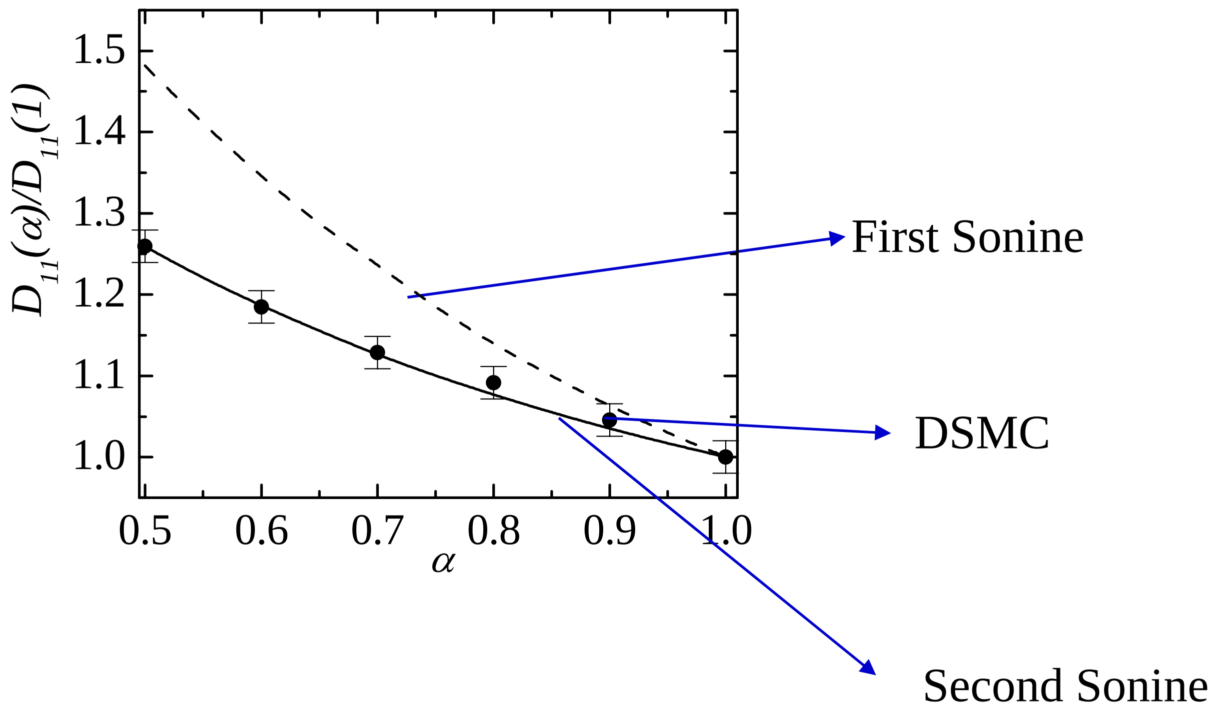

$$m_1/m_2 = 1/4; \sigma_1/\sigma_2 = 1/2; \phi = 0.2$$

$$\alpha_{22} = \alpha_{12} \equiv \alpha$$

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CONCLUSIONS

- Hydrodynamic equations for granular mixtures of inelastic hard spheres have been derived from the Enskog kinetic theory. A *normal* solution is obtained via the Chapman-Enskog method for states close to the local HCS

- **Exact** expressions for the equation of state, the cooling rate ζ, and the Navier-Stokes transport coefficients $\{D_{ij}, D_i^T, D_{ij}^F, \eta, \kappa, \lambda, D_{q,ij}, L_{ij}\}$.

- Explicit expressions for the kinetic and collisional contributions to ζ and transport coefficients are obtained by making an expansion in Sonine polynomials. All these coefficients are given in terms of the coefficients of restitution, masses, sizes, composition and density

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• Some analytical results are compared with numerical solutions of the RET in the cases od the tracer diffusion coefficient and the shear viscosity coefficient

• In general, the comparison shows good agreement between theory and simulation over a wide range of values of the parameters of the problem. This good agreement can be seen as an evidence of the *validity* of hydrodynamics to describe some states of granular fluids.

Thanks for your attention