DIFFUSION IN GRANULAR SHEAR FLOWS

Vicente Garzó
Departamento de Física,
Universidad de Extremadura, Badajoz

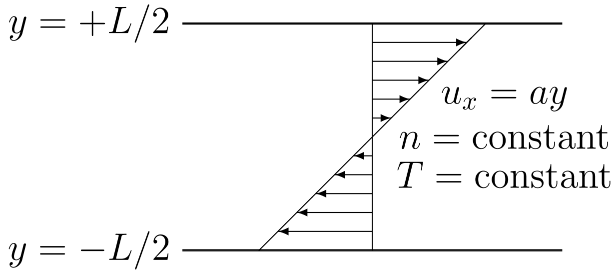
Granular Gases: Theory–Experiments–Simulations,
September 2–5, 2002.

OUTLINE

1. DESCRIPTION OF THE PROBLEM
2. GRANULAR GAS IN SIMPLE SHEAR FLOW
3. TRACER DIFFUSION IN SIMPLE SHEAR FLOW
4. CONCLUSIONS

THE PROBLEM

- Rapid granular flows → Fluid of hard spheres with *inelastic* collisions
- Simplest model: smooth hard spheres. Inelasticity characterized by a *constant* coefficient of normal restitution α.
- Due to the kinetic energy dissipation in collisions, energy must be externally injected to achieve stationary conditions. Mechanism of energy input: **Simple shear flow**.



- 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.

$$aP_{xy} = -\frac{d}{2}\zeta p, \quad \zeta \equiv \textit{cooling rate}$$

- Intrinsic connection between the velocity gradient (nonequilibrium parameter) and dissipation (restitution coefficient). Both parameters are not independent.

- PROBLEM: **Diffusion** of tracer particles (impurities) immersed in a granular fluid subjected to simple shear flow. Anisotropy of shear flow requires a diffusion tensor D_{ij} to describe the diffusion process. Campbell [J. Fluid Mech. (1997)] measured the elements of the self-diffusion tensor via molecular dynamics simulations.

- **Objective**: Determine the tracer diffusion tensor in granular shear flows by using a kinetic theory description→ Boltzmann kinetic equation for a granular binary mixture with one tracer component.

- System: **Granular gas** $\{m_2, \sigma_2, \alpha_{22}\}$+ **Impurities** $\{m_1, \sigma_1, \alpha_{12}\}$.

- Diffusion is induced in the system by a weak concentration gradient ∇x_1, with $x_1 = n_1/n_2$. Given that a is not necessarily small, the mass flux is modified by the presence of shear flow.

- Mass flux $\mathbf{j}_1$ of tracer particles:

$$j_{1,i} = -D_{ij}\nabla_j x_1,$$

  where D_{ij} depends on $\{m_1/m_2; \sigma_1/\sigma_2; \alpha_{22}; \alpha_{12}\}$.

GRANULAR GAS IN SIMPLE SHEAR FLOW

- Simple shear flow becomes spatially uniform in the local Lagrangian frame moving with the flow velocity $\mathbf{u}_2$: $f_2(\mathbf{r},\mathbf{v}) \to f_2(\mathbf{V})$, with $\mathbf{V}=\mathbf{v}-\mathbf{u}_2$.

$$-a_{ij}V_j\frac{\partial}{\partial V_i}f_2 = J_{22}[f_2,f_2], \quad a_{ij}=a\delta_{ix}\delta_{jy}$$

- Momentum transport: Pressure tensor

$$\mathbf{P}_2 = m_2\int d\mathbf{V}\mathbf{V}\mathbf{V}f_2$$

- Taking velocity moments in the Boltzmann equation:

$$a_{ik}P_{2,jk}+a_{jk}P_{2,ik} = m_2\int d\mathbf{V}V_iV_jJ_{22}[f_2,f_2] \equiv A_{ij}$$

- Closed problem once the collisional moment A_{ij} is known. This requires the explicit knowledge of f_2: formidable task!!

- Good estimate of the low velocity moments of $J_{22}[f_2,f_2]$ by using the leading Sonine approximation:

$$f_2(\mathbf{V}) \to f_{2,M}(\mathbf{V})\left[1+\frac{m_2}{2T_2}\left(\frac{P_{2,ij}}{n_2T_2}-\delta_{ij}\right)\left(V_iV_j-\frac{V^2}{d}\delta_{ij}\right)\right]$$

- Sonine predictions: Good agreement with Monte Carlo simulations.

TRACER DIFFUSION IN SIMPLE SHEAR FLOW

- Impurities obey a Boltzmann-Lorentz kinetic equation:

$$\partial_t f_1 - aV_y \frac{\partial}{\partial V_x} f_1 + (V_j + a_{ij} r_j) \frac{\partial}{\partial r_j} f_1 = J_{12}[f_1, f_2]$$

- Conservation law for the number density of tracer particles:

$$\left(\partial_t + a_{ij} r_j \frac{\partial}{\partial r_j}\right) x_1 + \frac{\nabla \cdot \mathbf{j}_1}{m_1 n_2} = 0,$$

- Mass flux

$$\mathbf{j}_1 = m_1 \int d\mathbf{V}\, \mathbf{V}\, f_1(\mathbf{V})$$

- Assuming that x_1 is slightly nonuniform,

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

- Each approximation $f_1^{(k)}$ is of order k in ∇x_1 but applies to arbitrary values of m_1/m_2, σ_1/σ_2 and is not restricted (a priori) to the quasielastic limit.

Reference state (absence of diffusion)

$$-aV_y\frac{\partial}{\partial V_x}f_1^{(0)}=J_{12}[f_1^{(0)},f_2],$$

- Partial pressure tensor

$$\mathbf{P}_1=m_1\int d\mathbf{v}\mathbf{V}\mathbf{V}f_1^{(0)}\equiv m_1\langle\mathbf{V}\mathbf{V}\rangle_1$$

- As done in the case of $\mathbf{P}_2$, I take the leading Sonine approximation of $f_1^{(0)}$:

$$f_1^{(0)}(\mathbf{V})\to f_{1,M}(\mathbf{V})\left[1+\frac{m_1}{2T_1}\left(\frac{P_{1,ij}}{n_1T_1}-\delta_{ij}\right)\left(V_iV_j-\frac{V^2}{d}\delta_{ij}\right)\right]$$

- Breakdown of energy equipartition

$$\gamma\equiv T_1/T_2=m_1\langle V^2\rangle_1/m_2\langle V^2\rangle_2\neq 1$$

- This nonequipartition has been oberved in real experiments of vibrated mixtures [Wildman and Parker, Phys. Rev. Lett. **88**, 064301 (2002); Feitosa and Menon, Phys. Rev. Lett. **88**, 198301 (2002)].

- The temperature ratio presents a complex depndence on

$$\{m_1/m_2;\sigma_1/\sigma_2;\alpha_{22};\alpha_{12}\}$$

First order (Diffusion tensor)

- First order of the expansion:

$$-aV_y \frac{\partial}{\partial V_x} f_1^{(1)} + J_{12}[f_1^{(1)}, f_2] = \frac{\partial f_1^{(0)}}{\partial x_1} \mathbf{V} \cdot \nabla x_1$$

- To determine the tracer diffusion tensor D_{ij}, similar approximations as those made before. First Sonine polynomial solution:

$$f_1^{(1)} \to -\frac{1}{n_1 T_1} f_{1,M} V_i D_{ij} \nabla_j x_1$$

- Elastic limit, $\alpha_{12} = \alpha_{22} = 1$, $D_{ij} = D_0 \delta_{ij}$, where D_0 is the tracer diffusion coefficient for a molecular gas.

- Influence of dissipation on the elements D_{ij} is in general quite important. Anisotropy induced in the gas by the shear flow. For instance, in the case of hard spheres ($d = 3$), $D_{xx} \neq D_{yy} \neq D_{zz}$ and $D_{xy} \neq D_{yx}$.

- Self-diffusion case: tracer particles are mechanicallly equivalent to the gas particles $\to m_1/m_2 = 1$, $\sigma_1/\sigma_2 = 1$, and $\alpha_{22} = \alpha_{12}$. In this case, the temperature ratio $\gamma = 1$. Behavior of D_{ij} is qualitatively similar to the one found in MD simulations of dense systems.

CONCLUSIONS

- Diffusion of impurities in a granular gas subjected to the simple shear flow. We are interested in the steady state where the effect of viscosity is compensated for by the dissipation in collisions. Due to anisotropy of shear flow, a diffusion tensor D_{ij} is required to describe the diffusion process. Low-density regime: Boltzmann kinetic theory.

- Rheological properties of the granular gas are well described by an approximate solution. Good agreement with Monte Carlo simulations.

- The theory predicts and the simulation confirms that the partial temperature of each species are different. The extent of the equipartition violation depends on the degree of dissipation and the mechanical differences of the particles.

- The kinetic theory results (based on the leading Sonine polynomial approximation) show that the influence of dissipation on the elements D_{ij} is quite significant. High anisotropy (diagonal elements are different) and cross–effects in the tracer diffusion. In the self-diffusion case, qualitative good agreement with MD simulations.

- Future work: Extension to dense systems by using the RET.