Diffusion and Dispersion in Flows of Granular Materials

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The big picture

"**Can we develop a general theory of the dynamics of turbulent flows and the motion of granular materials?** *So far, such 'nonequilibrium systems' defy the tool kit of statistical mechanics, and the failure leaves a gaping hole in physics.*" — "So Much More to Know ..." (2005)

- Motivation:
  - Flowing granular materials — a complex system far from equilibrium.
    - ★ No "general theory" but simple models can be enlightening.
  - Diffusion, rheology, etc. in/of granular flow are not well understood.

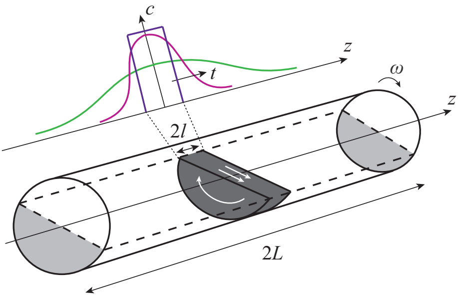
- Outline of the talk:
  1. Simple diffusion experiment with granular materials leads to anomalous scalings. Fundamentally new physics?
  2. Simple shear flow of a "granular continuum" can be addressed by a rheological model ⇒ new aspects to Taylor–Aris "dispersion"?

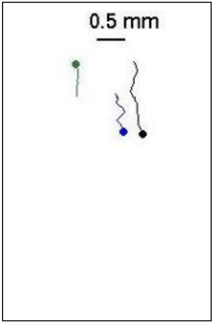
Diffusion of a "granular pulse" in a tumbler

- A band of colored particles in a monodisperse granular mixture diffuses axially as the container is rotated.

  (Lacey, *J. Appl. Chem.* 1954; Carley-Macauly & Donald, *Chem. Eng. Sci.* 1962)

- Many regimes of flow in a tumbler...restrict to continuous flow.
- Thin surface shear layer ⇒ velocity fluctuations ⇒ lateral diffusion.

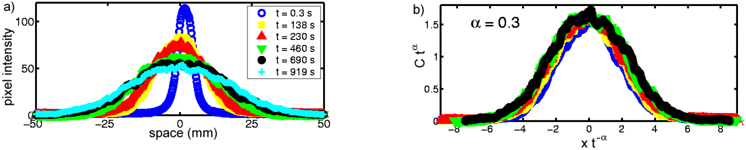




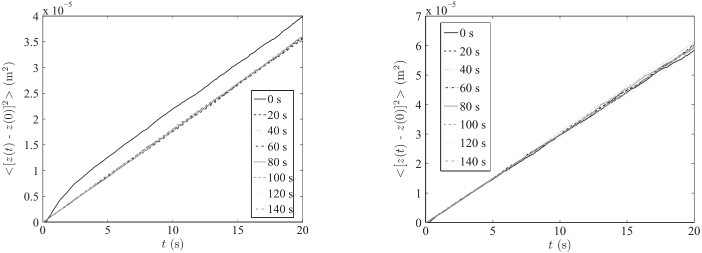
(Khan *et al.*, *New J. Phys.* 2011)

Anomalous macroscopic vs. normal microscopic scalings

- Experimental concentration profiles of an axially diffusing pulse of dyed black salt grains in white salt grains: (Khan & Morris, *Phys. Rev. Lett.* 2005)



- Mean square displacement (from simulations) vs time for a bed containing 25% small particles by volume: (Third *et al.*, *Phys. Rev. E* 2011)

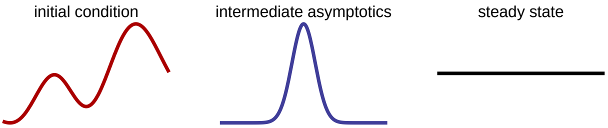


Intermediate asymptotics of diffusion

- Consider dimensionless diffusion equation

$$\frac{\partial C}{\partial T} = \frac{\partial}{\partial Z}\left(\mathcal{D}\frac{\partial C}{\partial Z}\right), \qquad \left.\frac{\partial C}{\partial Z}\right|_{Z=\pm 1} = 0, \quad C(Z,0) = C_i(Z).$$

- In general, we can have $\mathcal{D} = \mathcal{D}(C, Z, \cdots)$.
- $\mathcal{D} = 1$: random walk with $\langle(\Delta Z)^2\rangle \propto t$. (Einstein, *Ann. Phys.* 1905)
  - C-dependent jump probability leads to $\mathcal{D}(C)$. (Boon & Lutsko, *EPL* 2007)
- Similarity solution of the form $C(Z,T) = T^{-1/2}\mathfrak{C}(ZT^{-1/2})$.



(Barenblatt, *Scaling, Self-similarity, and Intermediate Asymptotics*, 1996)

Optimal self-similar solution

- Solutions for arbitrary initial data can be well-approximated (for $\mathcal{D} = 1$ and $T > T^*$) by the point-source similarity solution

$$C(Z,T) = \frac{1}{\sqrt{4\pi(T + T^*)}} \exp\left\{ -\frac{(Z + Z^*)^2}{4(T + T^*)} \right\}$$

provided that

$$Z^* = -\frac{M_1}{M_0}, \quad T^* = \frac{1}{2}\left[\frac{M_2}{M_0} - \left(\frac{M_1}{M_0}\right)^2 \right],$$

and $M_k := \int_{-\infty}^{+\infty} C_i(Z)\, Z^k \, \mathrm{d}Z$.

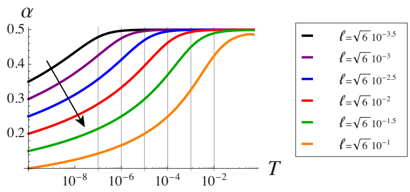
(Zel'dovich & Barenblatt, *Dokl. Akad. Nauk. SSSR* 1958)

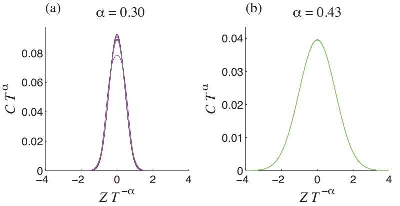
- Note: $Z^* = 0$ in this talk (symmetric initial conditions only).

Time-dependent anomalous collapse exponents

- Data collapses under rescaling $C(Z,T) \to C(Z/T^\alpha, T)T^\alpha$.
- $\Rightarrow$ we are balancing T^α with $\sqrt{T+T^*}$, meaning

$$\alpha(T) \simeq \frac{\ln(T+T^*)}{2\ln T} = \begin{cases} \frac{1}{\ln T}\left[\ln T^* + \frac{T}{2T^*} + \mathcal{O}(T^2)\right], & T \to 0, \\ \frac{1}{2} + \frac{1}{\ln T}\left[\frac{T^*}{2T} + \mathcal{O}(T^{-2})\right], & T \to \infty. \end{cases}$$





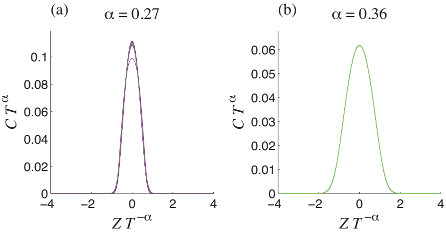
(Christov & Stone, *Proc. Natl Acad. Sci. USA* 2012)

Concentration-dependent diffusivity in bidisperse mixtures

- Suppose C is the concentration of larger particles, then $\mathcal{D}(C) = 1 + (C - 1/2)$. (Ristow & Nakagawa, *Phys. Rev. E* 1999)
- Seeking a self-similar solution $C(Z,T) = T^{-\alpha}\mathfrak{C}(\zeta)$ with $\zeta = T^{-\alpha}Z$:

$$0 = \mathfrak{C} + \zeta\mathfrak{C}' + \underbrace{\frac{(2 \mp 1)}{2\alpha} T^{1-2\alpha}\mathfrak{C}''}_{①} + \underbrace{\frac{1}{2\alpha} T^{1-3\alpha}\left(\mathfrak{C}^2\right)''}_{②}.$$

- If $\alpha = 1/3$, then $T^{1-2\alpha} = T^{1/3} \ll 1$ for $T \ll 1$.
- If $\alpha = 1/2$, then $T^{1-3\alpha} = T^{-1/2} \ll 1$ for $T \gg 1$.



Some open problems in granular diffusion

- Asymptotic solution matching across both scaling regimes in the nonlinear case? ⋆
- Account for disparate flow regimes (thin shear layer on top of bulk in solid body rotation)? (In progress, ICC & HAS.)
- Incorporate into axial segregation model? (Aranson & Tsimring, *Phys. Rev. Lett.* 1999)

(Khan *et al.*, *New J. Phys.* 2011)

Figure : evolution of mixture of 2/3 0.355–0.420 mm glass spheres and 1/3 small salt grains with 0.200–0.250 mm over 976 s (400 revolutions).

Enhanced macroscopic diffusion in shear flow

- Diffusive passive tracer advected by a flow in 2D obeys

$$\frac{\partial c}{\partial t} + v_x(y)\frac{\partial c}{\partial x} = \frac{\partial}{\partial x}\left(D\frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(D\frac{\partial c}{\partial y}\right).$$

- For $L/h \gg \overline{v_x}h/D_0$ and $|c'|/\bar{c} \ll 1$, can separate the evolution of the mean $\bar{c}$ from fluctuations c' to obtain a macrotransport equation:

$$\frac{\partial \bar{c}}{\partial t} + \overline{v_x}\frac{\partial \bar{c}}{\partial x} \approx \frac{\partial}{\partial x}\left(\bar{D}\frac{\partial \bar{c}}{\partial x}\right) - \overline{v_x'\frac{\partial c'}{\partial x}},$$

$$\frac{\partial}{\partial y}\left(D\frac{\partial c'}{\partial y}\right) \approx v_x'\frac{\partial \bar{c}}{\partial x}.$$

- NB: not 'dispersion' in the sense of wave-number-dependent phase speed, but in the sense of 'dispersal.'

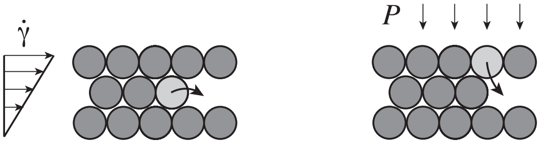
(Taylor, *Proc. R. Soc. A* 1953; Aris, *Proc. R. Soc. A* 1956;

Brenner & Edwards, *Macrotransport Processes*, 1993; Griffiths & Stone, *EPL* 2012)

Rheology of dense granular shear flow

- Dimensional analysis of pressure-controlled case leads us to

$$\text{Inertial number} \quad I = \frac{t_p = d\sqrt{\rho_p/P}}{t_{\dot\gamma} = 1/\dot\gamma} = \frac{\dot\gamma d}{\sqrt{P/\rho_p}}.$$



(a) mean deformation time $t_{\dot\gamma}$ (b) rearrangement time t_p

- Local rheology introduces a friction coefficient that depends on I:

$$\tau_{xy} = \mu(I)P, \qquad \mu(I) = \mu_0 + \frac{\mu_2 - \mu_0}{I_0/I + 1}, \qquad \phi(I) = \phi_0 + (\phi_2 - \phi_0)I.$$

- $\mu(0) = \mu_0$ "friction coefficient at yield" and $\mu(\infty) = \mu_2$ "maximum friction coefficient" for steady flow.

(Forterre & Pouliquen, *Annu. Rev. Fluid Mech.* 2008; Jop, Thèse De Doctorat 2006)

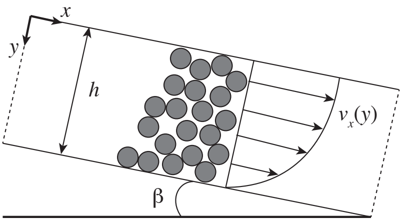
Example: granular material an inclined plane

- Flow commences if the Mohr–Coulomb yield criterion $|\tau_{xy}| > \mu P$ is satisfied:

$$\mu = \frac{|\tau_{xy}| = \phi\rho_p gy \sin\beta}{P = \phi\rho_p gy\cos\beta} \qquad \Rightarrow \qquad \mu = \tan\beta = const.$$

- Recall that local rheology is $\mu = \mu(I)$, so solve $\mu(I) = \tan\beta$ for I:

$$\frac{I}{I_0} \equiv \frac{(-\partial v_x/\partial y)d}{I_0\sqrt{\phi gy\cos\beta}} = \frac{\tan\beta - \mu_0}{\mu_2 - \tan\beta} \qquad \Rightarrow \qquad \frac{\partial v_x}{\partial y} = -A\sqrt{y}, \quad \underbrace{v_x(h) = 0}_{\text{“no slip”}}.$$



$$\boxed{v_x(y) = \frac{2}{3}A\left(h^{3/2} - y^{3/2}\right)}$$

“Bagnold profile”

(Bagnold, *Proc. R. Soc. Lond. A* 1954)

see also (Khakhar, *Macromol. Mater. Eng.* 2011)

Diffusivity of granular materials in shear flow

- Empirical model based on fitting to experimental data:

  (Hwang & Hogg, *Powder Technol.* 1980)

$$D = \underbrace{D_1}_{\text{“molecular”}} + \underbrace{D_2}_{\text{“shear-induced”}} \frac{\partial v_x}{\partial y}$$

- Somehow suspicious: no shear ($\partial v_x/\partial y = 0$) should $\Rightarrow$ no diffusivity ($D = 0$) since granular materials are non-Brownian.
- Kinetic theory for moderate ϕ up to ≈ 0.5 and perfect spheres:

  (Savage & Dai, *Mech. Mat.* 1993)

$$D = D_0 d^2 \left|\frac{\partial v_x}{\partial y}\right|, \qquad D_0(\phi, e) = \frac{d\sqrt{\pi T}}{8(1+e)\phi g_0(\phi)},$$

  where $g_0(\phi) = (2-\phi)/[2(1-\phi)^3]$ is the Carnahan–Starling radial distribution function at contact.
- But, we could've guessed this from dimensional analysis.

Taylor–Aris dispersion in granular shear flow on incline

- Assume Bagnold velocity $v_x(y) = \frac{5}{3}\overline{v_x}[1 - (y/h)^{3/2}]$ and Savage–Dai diffusivity $D = D_0 d^2 |\dot{\gamma}| = \frac{5}{2}\overline{v_x} D_0 d^2 \sqrt{y/h}$.
- Since ϕ-dependence in D is negligible (small variations in volume fraction in granular flow), this is a special case of Griffiths–Stone:

$$\frac{\partial \bar{C}}{\partial T} = \left(\frac{2}{3} + \frac{52}{4455} Pe^2\right) \frac{\partial^2 \bar{C}}{\partial \xi^2}, \qquad \xi = X - T.$$

- Compare to classical Taylor–Aris result for planar Couette flow:

$$\frac{\partial \bar{C}}{\partial T} = \left(1 + \frac{1}{180} Pe^2\right) \frac{\partial^2 \bar{C}}{\partial \xi^2}.$$

- $\dot{\gamma}$-dependence in D leads to some increase in the "dispersivity" $(52/4455 \approx 0.01 > 0.005 \approx 1/180)$?

Some open problems related to particle dispersal

- Restore ϕ-dependence in D, maybe using $\mu(I)$ & $\phi(I)$ local rheology?
  - NB: in Savage–Dai model $D(\phi) \sim 1/\phi + \mathcal{O}(1)$.
  - This is unlike $D(c) \sim c^n$ dependence in (Griffiths & Stone, *EPL* 2012).
- Consider non-local diffusive transport (fractional/anomalous diffusion). Is there an analogy to Taylor–Aris there?
- Work out other basic granular flows based on $\mu(I)$-rheology and then study dispersion? "Granular Poiseuille flow"?

Summary & conclusions

- What we have done:
  1. Showed that "anomalous" collapse exponents are possible under "normal" diffusion.
  2. Interpreted the latter in terms of Barenblatt's theory of intermediate self-similar asymptotics.
  3. Showed how to combine basic models for granular rheology (flow) and diffusion to study a canonical Taylor–Aris dispersion examples.

Thank you for your attention!

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