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.
- Many regimes of flow in a tumbler...restrict to continuous flow.
- Thin surface shear layer $\Rightarrow$ velocity fluctuations $\Rightarrow$ 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)

![Graph showing experimental concentration profiles](image)

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

![Graph showing mean square displacement](image)
Intermediate asymptotics of diffusion

- Consider dimensionless diffusion equation

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

- 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 \( C(Z, T) = T^{-1/2} \mathcal{C}(ZT^{-1/2}) \).

Optimal self-similar solution

- Solutions for arbitrary initial data can be well-approximated (for $D = 1$ 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 $M_k := \int_{-\infty}^{+\infty} C_i(Z) Z^k \, dZ$.


- Note: $Z^* = 0$ in this talk (symmetric initial conditions only).
Time-dependent anomalous collapse exponents

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

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

Concentration-dependent diffusivity in bidisperse mixtures

- Suppose $C$ is the concentration of larger particles, then
  \[ D(C) = 1 + (C - 1/2). \]  
  (Ristow & Nakagawa, Phys. Rev. E 1999)

- Seeking a self-similar solution $C(Z, T) = T^{-\alpha} c(\zeta)$ with $\zeta = T^{-\alpha} Z$:
  \[
  0 = c + \zeta c' + \frac{(2 + 1)}{2\alpha} T^{1-2\alpha} c'' + \frac{1}{2\alpha} T^{1-3\alpha} \left(c^2\right)''.
  \]

- 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.)

*(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:

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

\[ \frac{\partial}{\partial y} \left( D \frac{\partial c'}{\partial y} \right) \approx v'_x \frac{\partial \bar{c}}{\partial x}. \]

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

Rheology of dense granular shear flow

- Dimensional analysis of pressure-controlled case leads us to

\[
I = \frac{t_p}{t_\dot{\gamma}} = \frac{d \sqrt{\rho_p / P}}{1 / \dot{\gamma}} = \frac{\dot{\gamma} d}{\sqrt{P / \rho_p}}.
\]

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

\[
\tau_{xy} = \mu(I)P, \quad \mu(I) = \mu_0 + \frac{\mu_2 - \mu_0}{l_0/I + 1}, \quad \phi(I) = \phi_0 + (\phi_2 - \phi_0)I.
\]

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

Example: granular material an inclined plane

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

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

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

$$\frac{I}{I_0} \equiv \frac{(-\partial v_x/\partial y) d}{l_0 \sqrt{\phi g y \cos \beta}} = \frac{\tan \beta - \mu_0}{\mu_2 - \tan \beta} \Rightarrow \frac{\partial v_x}{\partial y} = -A \sqrt{y}, \quad v_x(h) = 0.$$  

"no slip"

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

"Bagnold profile"


see also (Khakhar, *Macromol. Mater. Eng.* 2011)
Diffusivity of granular materials in shear flow

- Empirical model based on fitting to experimental data:

\[
D = D_1 + D_2 \frac{\partial v_x}{\partial y}
\]

"molecular"  "shear-induced"

(Hwang & Hogg, Powder Technol. 1980)

- 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 \(\phi\) up to \(\approx 0.5\) and perfect spheres:

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

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 $v_x(y) = \frac{5}{3}v_x[1 - (y/h)^{3/2}]$ and Savage–Dai diffusivity $D = D_0 d^2 |\dot{\gamma}| = \frac{5}{2}v_x D_0 d^2 \sqrt{y/h}$.

- Since $\phi$-dependence in $D$ is negligible (small variations in volume fraction in granular flow), this is a special case of Griffiths–Stone:

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

- 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 \( \phi \)-dependence in \( D \), maybe using \( \mu(I) \) & \( \phi(I) \) local rheology?
  - NB: in Savage–Dai model \( D(\phi) \sim 1/\phi + O(1) \).
  - 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!
Selected Bibliography


- Christov & Stone, “Resolving a paradox of anomalous scalings in the diffusion of granular materials”

- Witelski & Bernoff, “Self-similar asymptotics for linear and nonlinear diffusion equations”

- Forterre & Pouliquen, “Flows of Dense Granular Media”

- Khakhar, “Rheology and Mixing of Granular Materials”