Continuum modeling of diffusion and dispersion in dense granular flows

Ivan C. Christov*,†, Howard A. Stone†

*Theoretical Division & Center for Nonlinear Studies, Los Alamos National Laboratory
†Mechanical & Aerospace Engineering, Princeton University

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Introduction: Taylor–Aris (shear) dispersion

Key physics:
- shear + diffusion = enhanced diffusion.

Applications
- measuring molecular diffusivity of solutes
- chromatography, separations
  (Golay, Gas Chromatography 1958)
- limits throughput and resolution in microfluidics
  (Bae et al., Lab Chip 2009)

What about granular shear flows?

“The transport process that leads to the spread of this cross-sectionally averaged temperature pulse turns out to resemble a pure axial conduction (or diffusion) process and is therefore called Taylor dispersion.” (Leal, Advanced Transport Phenomena, 2007, §3-H-2)
Theory of Taylor–Aris dispersion

- Diffusive passive tracer advected by a flow in 2D obeys
  \[
  \frac{\partial c}{\partial t} + \nu_x(z) \frac{\partial c}{\partial x} = \frac{\partial}{\partial x} \left( D \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial z} \left( D \frac{\partial c}{\partial z} \right).
  \]

- Let \( c(x, z, t) = \bar{c}(x, t) + c'(x, z, t) \) and \( \nu_x(z) = \bar{\nu}_x + \nu'_x(z) \).

- For \( L/h \gg \bar{\nu}_x h/D_0 \) and \( |c'|/\bar{c} \ll 1 \), can separate the evolution of the mean \( \bar{c} \) from fluctuations \( c' \) to obtain a macrotransport equation:
  \[
  \frac{\partial \bar{c}}{\partial t} + \bar{\nu}_x \frac{\partial \bar{c}}{\partial x} \approx \frac{\partial}{\partial x} \left( \bar{D} \frac{\partial \bar{c}}{\partial x} \right) - \nu'_x \frac{\partial c'}{\partial x},
  \]
  \[
  \frac{\partial}{\partial z} \left( D \frac{\partial c'}{\partial z} \right) \approx \nu'_x \frac{\partial \bar{c}}{\partial x}.
  \]

- NB: ‘dispersion’ in the sense of ‘dispersal’ (not \( \omega(k) \)).

Brenner & Edwards, Macrotransport Processes, 1993; Griffiths & Stone, EPL 2012)
Rapid granular flow down an inclined plane

- Pressure is “hydrostatic” through the layer $P = \phi \rho_p g (h - z) \cos \theta$.
- Steady flow for $\theta_2 > \theta > \theta_0 = \tan^{-1} \mu$.
- Volume fraction $\phi$ variations are negligible.
- Use your favorite local rheology (e.g., Forterre & Pouliquen, *Annu. Rev. Fluid Mech.* 2008),

$$\frac{\partial v_x}{\partial z} = \left\{ \frac{l_0}{d} \left( \frac{\tan \theta - \tan \theta_0}{\tan \theta_2 - \tan \theta} \right) \sqrt{\phi g \cos \theta} \right\} \sqrt{h - z}, \quad v_x(0) = 0. \quad \text{“no slip”}$$

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

Diffusivity of granular materials in shear flow

- **Empirical model based on fitting to experimental data:**

  \[ D = D_1 + D_2 \dot{\gamma}, \quad \dot{\gamma} \equiv \frac{\partial v_x}{\partial z}. \]


- **Somehow suspicious:** no shear \((\partial v_x/\partial z = 0)\) should \(\Rightarrow\) no diffusivity \((D = 0)\) since granular materials are non-Brownian.

- **Kinetic theory for perfect spheres and moderate \(\phi\) up to \(\approx 0.5:\)**

  \[ D = \chi d^2 |\dot{\gamma}|, \quad \chi = \chi(\phi, e) = \frac{d \sqrt{\pi T}}{8(1 + e)\phi g_0(\phi)}. \]


- **Also works in the dense flow regime, see G24.00003.**
Taylor–Aris dispersion in a granular shear flow

- Assume Bagnold profile $v_x(z) = \frac{5}{3} \sqrt{v_x} [1 - (1 - z/h)^{3/2}]$ and Savage–Dai diffusivity $D = D_0 \sqrt{1 - z/h}$, $D_0 = \frac{5}{2} \chi d^2 \frac{v_x}{h}$.

- Make dimensionless, introduce a Péclet number $Pe = \sqrt{v_x h / D_0}$, let $\epsilon = h/L$, and apply generalized Taylor–Aris for $D = D(z)$:

$$\frac{\partial \tilde{C}}{\partial T} = \left(1 + \frac{3}{55} Pe^2 \right) \frac{\partial^2 \tilde{C}}{\partial \xi^2}, \quad \xi = \frac{X - T}{\sqrt{3 Pe/(2 \epsilon)}}.$$

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

$$\frac{\partial \tilde{C}}{\partial T} = \left(1 + \frac{1}{30} Pe^2 \right) \frac{\partial^2 \tilde{C}}{\partial \zeta^2}, \quad \zeta = \frac{X - T}{\sqrt{Pe/\epsilon}}.$$

- Same order of magnitude: $3/55 \approx 0.055$, $1/30 \approx 0.033$. 
General shear profile

- Now, consider $\nu_x(z) = \left(\frac{1+\alpha}{\alpha}\right) \bar{v}_x [1 - (1 - z/h)^\alpha]$, $\alpha > 0$.

  For $\alpha < 1$, convex profile as in segregated bidisperse mixtures.
  
  (Wiederseiner et al., Phys. Fluids 2011; Fan et al., JFM 2014)

- Then, the Taylor–Aris dispersivity is

$$\frac{D}{D_0} = \begin{cases} 
\frac{1}{\alpha} \left[1 + \frac{\alpha}{2(4-\alpha)(4+\alpha)} Pe^2\right], & D \propto \dot{\gamma}, \\
1 + \frac{2}{3(9+9\alpha+2\alpha^2)} Pe^2, & D = \text{const}.
\end{cases}$$
Summary

- Derived the Taylor–Aris dispersivity for a general shear profile and a shear-rate dependent diffusivity:

\[
D = \frac{1}{\alpha} \left[ 1 + \frac{\alpha}{2(4 - \alpha)(4 + \alpha)} Pe^2 \right] \left[ (1 + \alpha) \frac{\bar{V}_x}{h} \chi d^2 \right]
\]

- To do:
  - Bidisperse mixtures; include segregation fluxes \( \propto S \dot{\gamma} (1 - c) c \).
  - Non-local effects for slow flows?


Thank you for your attention!