LA-UR-14-21335

Approved for public release; distribution is unlimited.

Title: Continuum modeling of diffusion and dispersion in dense granular flows

Author(s): Christov, Ivan C
Stone, Howard A

Intended for: American Physical Society March Meeting, 2014-03-03 (Denver, Colorado, United States)
Web

Issued: 2014-03-13 (rev.1)

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

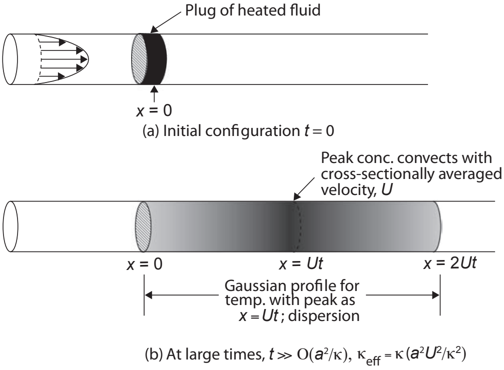
Focus Session: Continuum Description of Discrete Materials (A16.00005)

APS March Meeting 2014

Denver, Colorado

March 3, 2014

Introduction: Taylor–Aris (shear) dispersion



"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)

- Key physics: shear + diffusion = enhanced diffusion.
- Applications
  - measuring molecular diffusivity of solutes
    (Taylor, *Proc. R. Soc. A* 1954)
  - chromatography, separations
    (Golay, *Gas Chromatography* 1958)
  - limits throughput and resolution in microfluidics
    (Bae *et al.*, *Lab Chip* 2009)
- What about granular shear flows?

Los Alamos NATIONAL LABORATORY EST. 1943

Theory of Taylor–Aris dispersion

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

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

- Let $c(x,z,t) = \bar{c}(x,t) + c'(x,z,t)$ and $v_x(z) = \overline{v_x} + v_x'(z)$.
- 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:

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

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

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

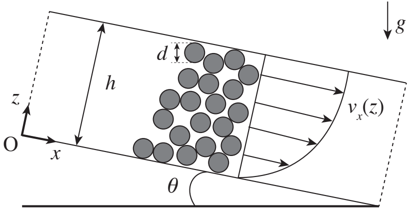
(Taylor, *Proc. R. Soc. A* 1953; Aris, *Proc. R. Soc. A* 1956;
Brenner & Edwards, *Macrotransport Processes*, 1993; Griffiths & Stone, *EPL* 2012)

Los Alamos NATIONAL LABORATORY EST. 1943

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 ϕ variations are negligible.
- Use your favorite local rheology (e.g., Forterre & Pouliquen, *Annu. Rev. Fluid Mech.* 2008),

$$\frac{\partial v_x}{\partial z} = \left\{ \frac{I_0}{d} \left(\frac{\tan\theta - \tan\theta_0}{\tan\theta_2 - \tan\theta} \right) \sqrt{\phi g \cos\theta} \right\} \sqrt{h-z}, \qquad \underbrace{v_x(0) = 0}_{\text{"no slip"}}.$$



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

"Bagnold profile" (Bagnold, *Proc. R. Soc. A* 1954)

Los Alamos NATIONAL LABORATORY EST. 1943

Diffusivity of granular materials in shear flow

- Empirical model based on fitting to experimental data:

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

$$D = \underbrace{D_1}_{\text{“molecular”}} + \underbrace{D_2}_{\text{“shear-induced”}} \dot{\gamma}, \qquad \dot{\gamma} \equiv \frac{\partial v_x}{\partial z}.$$

- 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 ϕ up to ≈ 0.5:

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

$$D = \chi d^2 \left|\dot{\gamma}\right|, \qquad \chi = \chi(\phi, e) = \frac{d\sqrt{\pi T}}{8(1+e)\phi g_0(\phi)}.$$

- Also works in the dense flow regime, see A16.00007.

Taylor–Aris dispersion in a granular shear flow

- Assume Bagnold profile $v_x(z) = \frac{5}{3}\overline{v_x}[1-(1-z/h)^{3/2}]$ and Savage–Dai diffusivity $D = D_0\sqrt{1-z/h}$, $D_0 = \frac{5}{2}\chi d^2\frac{\overline{v_x}}{h}$.
- Make dimensionless, introduce a Péclet number $Pe = \overline{v_x}h/D_0$, let $\epsilon = h/L$, and apply generalized Taylor–Aris for $D = D(z)$:

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

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

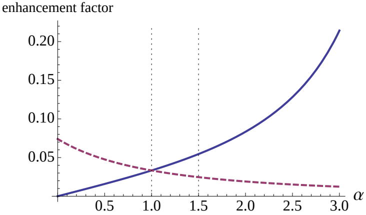
$$\frac{\partial \bar{C}}{\partial T} = \left(1 + \frac{1}{30}Pe^2\right)\frac{\partial^2 \bar{C}}{\partial \zeta^2}, \qquad \zeta = \frac{X-T}{\sqrt{Pe/\epsilon}}.$$

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

General shear profile

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

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



Summary

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

$$\boxed{\mathcal{D} = \frac{1}{\alpha}\left[1 + \frac{\alpha}{2(4-\alpha)(4+\alpha)} Pe^2\right]\left[(1+\alpha)\frac{\overline{v_x}}{h}\chi d^2\right]}$$

- To do:
  - Bidisperse mixtures; include segregation fluxes $\propto S\dot{\gamma}(1-c)c$.
  - Non-local effects for slow flows?
- Ref.: Christov & Stone, "Shear dispersion in dense granular flows," *Granular Matter*, to appear; arXiv:1402.6765.

Thank you for your attention!

DMS-1104047, CBET-1234500

LANL is operated by Los Alamos National Security, L.L.C. for the National Nuclear Security Administration of the U.S. Department of Energy under Contract No. DE-AC52-06NA25396.