Microstructure and Particle-Phase Stress in a Dense Suspension

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Predict microstructure and particle stresses in slow, steady, pure straining of a dense, single layer of spheres in a viscous fluid

Singh & Nott, J Fluid Mech. **412**, 279 (2000) Jenkins & La Ragione, J. Fluid Mech. **763**, 218 (2015)

Pure Straining



Area fraction: vAverage number of near contacts: k Short-range repulsive force: F_0 Elements of the Analysis

Pair translations and rotations

Pair forces and moments

Force and moment balances

Averages over directions and neighbors for equilibrium

Rate equations for the separation and orientation

Distribution of particle orientation and particle flux

Averaging over particle orientations for the stress

Kinematics

Treat BA exactly Relative velocity of centers of pair BA

$$\mathbf{v}_{\alpha}^{(BA)} = \frac{d}{dt} \mathbf{s}^{(BA)} \hat{\mathbf{d}}_{\alpha}^{(BA)} + 2a \frac{d}{dt} \boldsymbol{\theta}^{(BA)} \hat{\mathbf{t}}_{\alpha}^{(BA)}$$

Relative velocity of points of near contact of BA

$$\mathbf{v}_{\alpha}^{(BA)} + a\left(\boldsymbol{\omega}^{(A)} + \boldsymbol{\omega}^{(B)}\right) \hat{\mathbf{t}}_{\alpha}^{(BA)}$$

Treat nA on average Relative velocity of centers of pair nA

$$\mathbf{v}_{i}^{(nA)} = 2a\mathbf{D}_{\alpha\beta}\hat{\mathbf{d}}_{\beta}^{(nA)}$$

Relative velocity of points of near contact of nA

$$\mathbf{v}_{\alpha}^{(nA)} + a \boldsymbol{\omega}^{(A)} \hat{\mathbf{t}}_{\alpha}^{(nA)}$$

Interaction Forces

Jeffrey & Onishi (1984), Jeffrey (1992)

Pair BA

$$\begin{split} F_{\alpha}^{(BA)} &= 6\pi\mu a K_{\alpha\beta}^{(BA)} v_{\beta}^{(BA)} - \frac{F_{0}}{s^{(BA)}} \hat{d}_{\alpha}^{(BA)} - 9.54\pi\mu a^{2} \Big(\hat{t}_{\beta}^{(BA)} D_{\beta\gamma} \hat{d}_{\gamma}^{(BA)} \Big) \hat{t}_{\alpha}^{(BA)} \\ &+ \pi\mu a^{2} \bigg[\ln \bigg(\frac{a}{s^{(BA)}} \bigg) - 0.96 \bigg] \omega^{(A)} \hat{t}_{\alpha}^{(BA)} + \pi\mu a^{2} \ln \bigg(\frac{a}{s^{(BA)}} \bigg) \omega^{(B)} \hat{t}_{\alpha}^{(BA)} \\ &\quad K_{\alpha\beta}^{(BA)} &= \frac{1}{4} \frac{a}{s^{(BA)}} \hat{d}_{\alpha}^{(BA)} \hat{d}_{\beta}^{(BA)} + \frac{1}{6} \ln \bigg(\frac{a}{s^{(BA)}} \bigg) \hat{t}_{\alpha}^{(BA)} \hat{t}_{\beta}^{(BA)} \end{split}$$

$$\begin{aligned} \text{Pairs nA} \\ F_{\alpha}^{(nA)} &= 12\pi\mu a^2 K_{\alpha\beta}^{(nA)} D_{\beta\gamma} \hat{d}_{\gamma}^{(nA)} + \pi\mu a^2 \bigg[\ln \bigg(\frac{a}{\overline{s}} \bigg) - 0.96 \bigg] \omega^{(A)} \hat{t}_{\alpha}^{(nA)} \\ &- \frac{F_0}{\overline{s}} \hat{d}_{\alpha}^{(nA)} + 2\pi\mu a^2 \bigg[\ln \bigg(\frac{1}{\overline{s}} \bigg) - 0.96 \bigg] \Big(\hat{t}_{\beta}^{(nA)} D_{\beta\gamma} \hat{d}_{\gamma}^{(nA)} \Big) \hat{t}_{\alpha}^{(nA)} \\ &K_{\alpha\beta}^{(nA)} &= \frac{1}{4} \frac{a}{\overline{s}} \hat{d}_{\alpha}^{(nA)} \hat{d}_{\beta}^{(nA)} + \frac{1}{6} \ln \bigg(\frac{a}{\overline{s}} \bigg) \hat{t}_{\alpha}^{(nA)} \hat{t}_{\beta}^{(nA)} \end{aligned}$$

Force Balance, Particle A

$$F_{\alpha}^{(BA)} + \sum_{n \neq B}^{N^{(A)}} F_{\alpha}^{(nA)} = 0$$

$$F_{\alpha}^{(AB)} = -F_{\alpha}^{(BA)}, \ \hat{d}_{\alpha}^{(AB)} = -\hat{d}_{\alpha}^{(BA)}, \ \hat{t}_{\alpha}^{(AB)} = -\hat{t}_{\alpha}^{(BA)}$$

Difference of force balances

Normal component

$$0 = 3\pi\mu a \frac{a}{s^{(BA)}} \frac{d}{dt} s^{(BA)} - 2 \frac{F_0}{s^{(BA)}}$$

$$+ 6\pi\mu a^2 \frac{a}{\overline{s}} \hat{d}_{\alpha}^{(BA)} J_{\alpha\beta\gamma} D_{\beta\gamma} - 2 \frac{F_0}{\overline{s}} Y_{\alpha} \hat{d}_{\alpha}^{(BA)}$$
Tangential component

$$0 = 4\pi\mu a^2 \left[\ln\left(\frac{a}{s^{(BA)}}\right) + 3.84 \right] \frac{d}{dt} \theta^{(BA)} - 19\pi\mu a^2 \hat{t}_{\alpha}^{(BA)} D_{\alpha\beta} \hat{d}_{\beta}^{(BA)}$$

$$+ \pi\mu a^2 \left[2\ln\left(\frac{a}{s^{(BA)}}\right) - 0.96 \right] S + 6\pi\mu a^2 \frac{a}{\overline{s}} \hat{t}_{\alpha}^{(BA)} J_{\alpha\beta\gamma} D_{\beta\gamma}$$

$$(S = \omega^A + \omega^B)$$

Moment Balance, Particle A

$$\varepsilon_{\alpha\beta}F_{\alpha}^{(BA)}\hat{d}_{\beta}^{(BA)} + \varepsilon_{\alpha\beta}\sum_{n\neq B}^{N^{(A)}}F_{\alpha}^{(nA)}\hat{d}_{\beta}^{(nA)} = 0$$

 $(\varepsilon_{12} = -\varepsilon_{12} = 1, \varepsilon_{11} = \varepsilon_{22} = 0)$

Sum of Moment Balances

$$0 = 2 \left[\ln \left(\frac{a}{s^{(BA)}} \right) + 3.84 \right] \frac{d}{dt} \theta^{(BA)} - 9.54 \hat{t}_{\alpha}^{(BA)} D_{\alpha\beta} \hat{d}_{\beta}^{(BA)} + \left[\ln \left(\frac{a}{s^{(BA)}} \right) + \frac{k-1}{2} \ln \left(\frac{a}{\overline{s}} \right) \right] S + 2 \left[\ln \left(\frac{a}{\overline{s}} \right) - 0.96 \right] \varepsilon_{\beta\gamma} A_{\alpha\beta} D_{\alpha\gamma}$$

Neighborhood Averages

Isotropic representations

$$\mathbf{Y}_{\alpha} \equiv \overline{\sum_{n \neq B}^{\mathbf{N}^{(A)}} \hat{\mathbf{d}}_{\alpha}^{(nA)}} = \boldsymbol{\xi} \hat{\mathbf{d}}_{\alpha}^{(BA)}$$

$$\mathbf{A}_{\alpha\beta} \equiv \overline{\sum_{\mathbf{n}\neq\mathbf{B}}^{\mathbf{N}^{(A)}} \hat{\mathbf{d}}_{\alpha}^{(\mathbf{n}A)}} \hat{\mathbf{d}}_{\beta}^{(\mathbf{n}A)} = \beta_1 \delta_{\alpha\beta} + \beta_2 \hat{\mathbf{d}}_{\alpha}^{(\mathbf{B}A)} \hat{\mathbf{d}}_{\beta}^{(\mathbf{B}A)}$$

$$\begin{split} \mathbf{J}_{\alpha\beta\gamma} &\equiv \overline{\sum_{n\neq B}^{\mathbf{N}^{(A)}} \hat{d}_{\alpha}^{(nA)} \hat{d}_{\beta}^{(nA)}} \hat{d}_{\gamma}^{(nA)}} \\ &= \left[\alpha_{1} \hat{d}_{\alpha}^{(BA)} \hat{d}_{\beta}^{(BA)} \hat{d}_{\gamma}^{(BA)} \right. \\ &\quad + \alpha_{2} \left(\delta_{\alpha\beta} \hat{d}_{k}^{(BA)} + \delta_{\alpha\gamma} \hat{d}_{\beta}^{(BA)} + \delta_{\beta\gamma} \hat{d}_{\alpha}^{(BA)} \right) \right] \end{split}$$

Neighborhood Averages

$$\frac{\overline{\mathbf{s}}}{a} = \frac{\sqrt{\pi}}{8\mathbf{v}\mathbf{g}_0} \qquad \mathbf{g}_0 = \frac{16 - 7\mathbf{v}}{16(1 - \mathbf{v})^2}$$

Isotropic distribution function

$$\overline{\Psi_{\alpha..\gamma}} = 2\int_{0}^{\pi} I(\theta') \hat{d}_{\alpha}..\hat{d}_{\gamma} d\theta'$$

$$I(\theta') = \begin{cases} 0, & 0 < \theta' < \pi / 3 \\ 3(k-1) / 4\pi, & \pi / 3 < \theta' < \pi \end{cases}$$

$$\alpha_1 = 0, \quad \alpha_2 = -\frac{3\sqrt{3(k-1)}}{16\pi} \equiv \alpha$$

$$\beta_1 = \frac{(k-1)}{2} + \frac{3\sqrt{3}(k-1)}{16\pi}, \quad \beta_2 = -\frac{3\sqrt{3}(k-1)}{8\pi} = 2\alpha$$
$$\xi = -\frac{3\sqrt{3}(k-1)}{4\pi} = 4\alpha$$

Trajectory Equations

$$D_{\alpha\beta} = \begin{bmatrix} \dot{\gamma} & 0\\ 0 & -\dot{\gamma} \end{bmatrix} \qquad \hat{d}_{\alpha}^{(BA)} = (\sin\theta, \cos\theta)$$
$$\hat{d}_{\alpha}^{(BA)} D_{\alpha\beta} \hat{d}_{\beta}^{(BA)} = -\dot{\gamma}\cos 2\theta, \qquad \hat{t}_{\alpha}^{(BA)} D_{\alpha\beta} \hat{d}_{\beta}^{(BA)} = \dot{\gamma}\sin 2\theta$$

Lengths dimensionless by a and $F \equiv F_0 / (\pi \mu a^3 \dot{\gamma})$

$$\frac{1}{s}\frac{\mathrm{d}s}{\mathrm{d}\gamma} = \frac{2}{3}F\left(\frac{1}{s} + 4\frac{\alpha}{\overline{s}}\right) + 4\frac{\alpha}{\overline{s}}\cos 2\theta$$
$$\left[\ln\left(\frac{1}{s}\right) + 3.84\right]\frac{\mathrm{d}\theta}{\mathrm{d}\gamma} = \left(4.77 - 3\alpha\frac{1}{\overline{s}}\right)\sin 2\theta - \frac{1}{2}\ln\left(\frac{1}{s}\right)S$$

Tangential force difference - Sum moments

$$\mathbf{S} = -\frac{12\alpha}{(4\alpha - k + 1)} \frac{1/\overline{s}}{\ln(1/\overline{s}) - 0.96} \sin 2\theta$$

Contact Distribution

 $A(\theta)d\theta$: number of contacts within $d\theta$

$$A(\theta)\frac{d\theta}{d\gamma} = \text{constant and } \int_0^{\pi/2} A(\theta)d\theta = \frac{k}{4}$$

Knowledge of k determines the constant of integration.

Implement as differential equations

$$I(\theta) \equiv \int_0^{\theta} A(\theta') d\theta'$$

 $\frac{dI}{d\theta} = A, \quad I(0) = 0, \quad I(\pi/2) = k/4$ $\frac{dA}{d\theta} = -\frac{A}{\dot{\theta}}\frac{d\dot{\theta}}{d\theta} \quad \frac{d\dot{\theta}}{d\theta} = \frac{\partial\dot{\theta}}{\partial\theta} + \frac{\partial\dot{\theta}}{\partial s}\frac{ds}{d\theta}$

Differential Equations

$$\frac{\mathrm{d}\mathbf{s}}{\mathrm{d}\theta} = \frac{\mathrm{d}\mathbf{s} / \mathrm{d}\gamma}{\mathrm{d}\theta / \mathrm{d}\gamma} \equiv \mathrm{f}[\mathbf{s}, \theta; \overline{\mathbf{s}}(\nu), k]$$

$$\frac{dA}{d\theta} = \frac{A}{d\theta / d\gamma} \left[\frac{\partial}{\partial \theta} \left(\frac{d\theta}{d\gamma} \right) + \frac{\partial}{\partial s} \left(\frac{d\theta}{d\gamma} \right) \frac{ds}{d\theta} \right]$$
$$\frac{dI}{d\theta} = A$$
$$\frac{d\gamma}{d\theta} = \frac{1}{d\theta / d\gamma}$$

Boundary Conditions

 $0 \le x \le 1 \qquad \theta = \theta_0 + (\theta_1 - \theta_0) x$ $s(\theta_0) = 0.003 \qquad s(\theta_1) = 0.003$ $I(\theta_0) = 0 \qquad I(\theta_1) = k/4$ $\gamma(\theta_0) = 0 \qquad \gamma(\theta_1) = 1.1$

Separation

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The repulsive force creates asymmetry about $\pi/4$.

Inverse Separation



The asymmetry of the separation clarified.

Angular Velocity



 $A(\theta)\frac{d\theta}{d\gamma} = \text{ constant}$

Circumferential Distribution



The repulsive force shifts the anisotropy due to the flow, symmetric about $\pi/4$, to a distribution that is asymmetric.

Circumferential Distribution



Asymmetry about $\pi/4$ in both the distribution and interval.

Stress (dimensional)

$$T_{\alpha\beta} = na \int_{0}^{2\pi} \mathbf{A}(\boldsymbol{\theta}) \mathbf{F}_{\alpha}^{(BA)} \hat{\mathbf{d}}_{\beta}^{(BA)} d\boldsymbol{\theta}$$

n: number/area

$$F_{\alpha}^{(BA)} = -\sum_{n \neq B}^{N^{(A)}} F_{\alpha}^{(nA)}$$
$$t_{\alpha\beta} = \frac{T_{\alpha\beta}}{a\mu\dot{\gamma}}, \quad n = \frac{\nu}{\pi a^2}, \quad F = \frac{F_0}{\pi a^3\mu\dot{\gamma}}$$

$$t_{\alpha\beta} = v \frac{\alpha}{\overline{s}} \int_{0}^{2\pi} A(\theta) \left(4F + 6\cos 2\theta \right) \hat{d}_{\alpha} \hat{d}_{\beta} d\theta$$

+ $v \left(9.54 - \frac{6}{\overline{s}} \right) \alpha \int_{0}^{2\pi} A(\theta) \sin 2\theta \hat{t}_{\alpha} \hat{d}_{\beta} d\theta$
+ $v \frac{12\alpha}{(3\alpha - k + 1)} \frac{1/\overline{s}}{\ln(1/\overline{s})} \int_{0}^{2\pi} A(\theta) \ln\left(\frac{1}{s}\right) \sin 2\theta \hat{t}_{\alpha} \hat{d}_{\beta} d\theta$

$$\hat{d}_{\alpha}^{(AB)} = (\sin\theta, \cos\theta), \ \hat{t}_{\alpha}^{(AB)} = (\cos\theta, -\sin\theta)$$

Pressure

$$p \equiv -\frac{1}{2}(t_{xx} + t_{yy})$$

$$p = -4\nu \frac{\alpha}{\overline{s}} \int_0^{\pi/2} A(\theta) (2F + 3\cos 2\theta) d\theta$$

Shear stress

$$\tau \equiv \frac{1}{2} (t_{xx} - t_{yy})$$

$$\tau = -4\nu \frac{\alpha}{\overline{s}} \int_{0}^{\pi/2} A(\theta) (2F + 3\cos 2\theta) \cos 2\theta d\theta$$
$$+\nu \left(4.77 - \frac{3\alpha}{\overline{s}} \right) \int_{0}^{2\pi} A(\theta) \sin^{2} 2\theta d\theta$$
$$+\nu \frac{6\alpha}{(3\alpha - k + 1)} \frac{1/\overline{s}}{\ln(1/\overline{s})} \int_{0}^{2\pi} A(\theta) \ln\left(\frac{1}{s}\right) \sin^{2} 2\theta d\theta$$

Stresses



Asymmetry about $\pi/4$ creates particle pressure.

Initial/Final Separation



The initial/final separation of the "typical" trajectory is where the shear stress exhibits a maximum (0.003).

Conclusions

A rough implementation of particle equilibrium for particles assumed to interact as pairs through points of near contact produces expressions for the normal and tangential components of their relative velocities as functions of their orientation with respect to the flow.

From these velocities, the separation of neighboring particles and their circumferential distribution can be determined as functions of orientation.

The existence of asymmetries in the circumferential distribution of particles influences the shear stress and produces a pressure associated with viscous interactions between particle pairs at points of near contact.