ORIENTATIONAL TRANSPORT AND TRANSIENT OF ORIENTED GRAINS

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Rheology of oriented grains

The microscopic orientation of oriented grains (prolate to oblate) plays an important role in their macroscopic rheological response



Orientational transport - vibrating boundaries

It was observed that elongated grains agitated by vibrating boundaries tend to align with the non-vibrating boundaries



 $l/d = \{1/6(\mathbf{\nabla}), 1/4(\mathbf{\Delta}), 1/2(\mathbf{\Box}), 1/1(\mathbf{O}), 2/1(\mathbf{\Box}), 4/1(\mathbf{\Delta}), 6/1(\mathbf{\nabla})\}$

A first order macroscopic representation of the microscopic orientation is

 $\mathbf{A} = \frac{1}{N} \sum_{i=1}^{N} \mathbf{k}_{i} \otimes \mathbf{k}_{i} \quad , \quad \mathbf{A}' = \mathbf{A} - \mathbf{I}/3 \quad , \quad \mathbf{S} = \sqrt{3/2 \left(\mathbf{A}' : \mathbf{A}'\right)}$

It is identified that the significant deviation of the macroscopic shear viscosity of oriented grains is related to the microscopic orientation and alignment



To account for the microscopic orientation, a simple (but effective) extension is proposed as

 $\boldsymbol{\sigma} = (p - \lambda \operatorname{tr} \mathbf{D}) \mathbf{I} - 2\eta \left[\mathbf{D}' - 3\alpha \left(\mathbf{D}' \mathbf{A}' + \mathbf{A}' \mathbf{D}' - 2/3 (\mathbf{D}' : \mathbf{A}') \mathbf{I} \right) \right]$

where the pressure p, bulk viscosity λ and shear viscosity η depend on the velocity fluctuations (granular temperature) and are taken from kinetic theory of spherical grains. The phenomenological parameter $\alpha \leq 1$, which accounts for the dependency of the shear viscosity on the microscopic orientation, is a function of the "surface" properties of the grains and takes the value $\alpha = 1$ for frictionless cylindrical grains.

which can be attributed to orientational transport. At steady-state the orientational balance law and boundary conditions are

 $-\psi\sqrt{T}/d_v \mathbf{A}' + \nabla \cdot \left(\beta\sqrt{T}/d_v \nabla \mathbf{A}'\right) = \mathbf{0} \quad , \quad \sqrt{T}/d_v \left(\nabla \mathbf{A}' \cdot \mathbf{n}\right) = \beta_b \left[\mathbf{A}'_b - \mathbf{A}'\right]$

The orientation and granular temperature fields are



for $e_n = 0.9$ and $e_n = 0.7$ respectively, where the granular temperature fields are taken from kinetic theory of spherical grains and

 $\psi = 0.2\nu^{-3.5} (1 - |r_g|)^{2.55}$, $\beta = c_1\nu$, $\beta_b = c_2\nu$, $r_g = 0.8$, $c_1 = 1$, $c_2 = 1$

Orientation of oriented grains

As the microscopic orientation plays a significant role in the macroscopic response, it is introduced into the formulation as an additional field, orientational tensor A, governed by a balance law. A balance law has the general form

$$\dot{\mathbf{A}} = \mathbf{P} + \nabla \cdot \mathbf{G}$$

where \mathbf{P} is the orientational production (and volumetric supply) and \mathbf{G} is the non convective orientational flux that need to be specified by constitutive laws.

Orientational production

For homogenous steady-state flows where $\dot{A}=0, \ \nabla\cdot G=0 \Rightarrow P=0,$ the production is proposed as

 $\mathbf{P} = \mathbf{W}\mathbf{A} - \mathbf{A}\mathbf{W} + \phi \left[\mathbf{A}\mathbf{D} + \mathbf{D}\mathbf{A} - 2(\mathbf{A}:\mathbf{D})\mathbf{A}\right] - \psi \sqrt{T}/d_v \mathbf{A}'$

The phenomenological parameters are function of the solid volume fraction and the aspect ratio

 $|\phi(r_g,\ldots)| \le 1 \quad , \quad \psi(\nu;r_g,\ldots) \ge 0$

where d_v is the size and $r_g = (l - d)/(l + d)$ is the aspect ratio of a grain.

This suggests strong dependency of the orientation field on the granular temperature field and the boundary conditions.

Orientational transient

Under homogenous shear reversal and the generalized inertia rheology

$$\dot{\mathbf{A}} = \mathbf{W}\mathbf{A} - \mathbf{A}\mathbf{W} + \phi \left[\mathbf{A}\mathbf{D} + \mathbf{D}\mathbf{A} - 2(\mathbf{A}:\mathbf{D})\mathbf{A}\right] - \psi \|\mathbf{D}\|\mathbf{A}'$$

 $\boldsymbol{\sigma} = p\mathbf{I} - p\mu(I) \left[\bar{\mathbf{D}}' - 3\alpha \left(\bar{\mathbf{D}}'\mathbf{A}' + \mathbf{A}'\bar{\mathbf{D}}' - 2/3(\bar{\mathbf{D}}':\mathbf{A}')\mathbf{I} \right) \right]$

when taking $\sqrt{T}/d_v \approx ||\mathbf{D}||$, we observe complex strain hardening response due to transient microscopic orientation rearrangement



Directional arrest can occur, if the applied shear traction is insufficient to overcome the strain hardening. At arrested configuration, a second shear reversal may yield strain softening (and potentially resume of flow) or additional strain hardening which suggests strong amplitude dependency of shear oscillations.

Orientational transport

The orientational flux is proposed to take the simple form

 $\mathbf{G} = \beta \sqrt{T} / d_v \nabla \mathbf{A}'$

and the associated boundary conditions are

 $\sqrt{T}/d_v \left(\nabla \mathbf{A}' \cdot \mathbf{n} \right) = \beta_b \left[\mathbf{A}'_b - \mathbf{A}' \right] \quad \text{or} \quad \sqrt{T}/d_v \left(\nabla \mathbf{A}' \cdot \mathbf{n} \right) = \beta_b \left(\mathbf{A}'_b : \mathbf{A}' \right) \left[\mathbf{A}'_b - \mathbf{A}' \right]$

where \mathbf{A}'_b is the orientation of the boundary and the phenomenological parameters $\beta(\nu; r_q, ...) \ge 0$, $\beta_b(\nu; r_q, ...) \ge 0$

characterizing the orientational flux from "high" alignment toward "low" alignment, with the properties

$$\beta \to 0$$
 , $\beta_b \to 0$ for $r_g \to 0$ or $\nu \to 0$

Conclusions and future work

The complexity of the microscopic orientational response of oriented grains is still not well understood with limited treatment using continuum framework. More work if required to advance our understanding of the underlaying physics using DEM simulations and experiments which will contribute to the formulation of continuum theory of oriented granular materials.

Two research directions are identified:

- The construction of orientational flux and boundary conditions supported by DEM and experimental data
- Generalization of the balance of fluctuation kinetic energy to orientated grains that includes the dependency on the microscopic orientation and the aspect ratio