A simple generalization of kinetic theory for granular flows of non-spherical, oriented particles

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We generalize kinetic theory of inelastic spheres to uniaxial, non-spherical grains, by including the orientational tensor as a state variable. The theory has one phenomenological parameter to account for the dependency of the stresses on the orientation, which is exactly one for frictionless cylinders. We model the competition between the alignment induced by shearing and the misalignment due to collisions in the evolution law for the orientational tensor. The theory can predict the significant reduction in the viscosity in response to alignment measured in discrete simulations of homogeneous shear flows of prolate and oblate frictionless cylinders.

Kinetic theory of granular gases [14, 19] provides an effective continuum approach to study granular systems over a wide range of densities, loading and geometries, specifically under inhomogeneous flow conditions, where the boundaries play an important role [16, 31]. While this approach proved to be advantageous and accurate, it was developed by considering binary collisions of spheres, avoiding the additional complexity associated with the mutual orientation of non-spherical particles. Recent discrete numerical simulations suggest that the orientation of axisymmetric grains, which is governed by their shape, is crucial in determining their rheological response [5, 6, 24, 30]. In particular, at least in the case of cylinders, while alignment does not significantly affect the isotropic component of the stress tensor, the particle pressure, it can yield up to one order of magnitude reduction in the shear stress.

In this letter, we generalize the kinetic theory of granular gases to uniaxial grains, by including the orientational order, described though a tensor, as an additional state variable in the constitutive law of the stress tensor. Alignment and its coupling to the stresses have been the subject of intense research activity on molecular liquid crystals, random assemblies of non-spherical molecules that can show preferential orientation in response to change in temperature, concentration and/or when subjected to external fields [12, 13, 18, 25, 27]. Granular, non-spherical particles, for which Brownian motion is irrelevant, tend to align in response to shearing, while interparticle, inelastic collisions are expected to randomize the particle alignment. Hence, the intensity of the particle agitation should be explicitly included in the evolution law of the orientation.

Uniaxial, convex particles, such as cylinders, spherocylinders, or ellipsoids, can be at a minimum characterized by their length, l, along the axis of symmetry and by their maximum extension, d, in the plane perpendicular to the axis of symmetry. Here, we define them through the equivalent diameter, d_v, i.e., the diameter of a sphere of equivalent volume, and their aspect ratio, $r_g = (l-d)/(l+d)$, which gives $r_g = 0$ for $l = d$, $0 < r_g < 1$ for $l > d$ (prolate grains), and $-1 < r_g < 0$ for $l < d$ (oblate grains) – see Fig. 1(a). The orientation of an uniaxial grain is defined by the dyad $(\mathbf{k}\otimes\mathbf{k})$, where $\mathbf{k}$ is the direction of the particle symmetry axis. For assembly of particles, the averaged orientational tensor takes the form

$$\mathbf{A} = \frac{1}{N}\sum_{i=1}^{N}(\mathbf{k}_i\otimes\mathbf{k}_i)\ , \tag{1}$$

where N is number of particles, and $(\mathbf{k}_i\otimes\mathbf{k}_i)$ is the orientation of the i-th grain. The orientational tensor is symmetric, positive semidefinite, has unit trace, $\mathrm{tr}\,\mathbf{A} = 1$, and two nonlinear invariants. It is convenient to define the deviation from isotropic orientation as $\mathbf{A}' = \mathbf{A} - \mathbf{I}/3$. Here, we define a scalar measure of the orientation, $0 \geq S \geq 1$, as the largest eigenvalue of the tensor $3/2\mathbf{A}'$, and the director, $\mathbf{u}$, the average direction of the particle axis of symmetry in the case of preferential alignment, as the associate eigenvector [8]. The measure S vanishes in the absence of alignment ($\mathbf{A}' = \mathbf{0}$) and equals one for perfectly aligned grains ($\mathbf{A}' = \mathbf{u}\otimes\mathbf{u} - \mathbf{I}/3$).

For granular materials composed of identical, hard spheres of mass density ρ_p and diameter d_v, the hydrodynamic fields of a linear kinetic theory (in which the stresses are at first order in the spatial gradients [15]) are the solid volume fraction, ν, the mean velocity, $\mathbf{v}$ and the granular temperature, T, one-third of the mean square of the particle velocity fluctuations. The latter represents the measure of the particle agitation. The kinematics is determined by the quantity $\mathbf{L} = \nabla\mathbf{v}$, the velocity gradient, which is decomposed into its skew-symmetric part, the vorticity $\mathbf{W} = (\mathbf{L} - \mathbf{L}^T)/2$, and its symmetric part, the rate of deformation $\mathbf{D} = (\mathbf{L}+\mathbf{L}^T)/2$. $\mathbf{D}' = \mathbf{D} - (\mathrm{tr}\,\mathbf{D}/3)\mathbf{I}$ is the deviatoric part of the rate of deformation. Solution to the Enskog model for inelastic, hard spheres at first order in the spatial gradients (Navier-Stokes approximation) provides the following expression for the stress tensor [14]

$$\boldsymbol{\sigma} = (p - \lambda\,\mathrm{tr}\,\mathbf{D})\,\mathbf{I} - 2\eta\mathbf{D}', \tag{2}$$

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where: p is the hydrostatic pressure; λ and η are the volumetric and the shear viscosities, respectively. The expression for the shear viscosity is

$$\eta = \frac{8J\nu^2 g_0}{5\pi^{1/2}} \rho_p d_v T^{1/2}, \tag{3}$$

where: J is a known function [2] of the coefficient of normal restitution, e_n (the negative of the ratio of post- to pre-collisional, normal relative velocity between colliding grains, here taken to be a constant), and the solid volume fraction [21]; and g_0 is the radial distribution function at contact [29], which is also a known function [1] of the solid volume fraction ν and is singular at the critical value $\nu = \nu_c$, at which the average interparticle distance, at least along the direction of principal compression, vanishes [7]. The critical volume fraction decreases with increasing coefficient of sliding friction, μ, and corresponds to the minimum volume fraction at which rate-independent components of the stresses develop in the case of soft spheres [11, 28]. Expressions for the pressure and the volumetric viscosity can also be found in [14].

For granular materials composed of identical, hard, uniaxial, non-spherical grains, we generalize Eq. (2) to include a linear dependency on the orientational tensor into the deviatoric part of the stress tensor [22]

$$\begin{aligned}\boldsymbol{\sigma} &= (p - \lambda \operatorname{tr} \mathbf{D})\, \mathbf{I} \\ &\quad - 2\eta \left[\mathbf{D}' - 3\alpha \left(\mathbf{D}'\mathbf{A}' + \mathbf{A}'\mathbf{D}' - 2/3(\mathbf{D}' : \mathbf{A}')\mathbf{I}\right)\right], \end{aligned}\tag{4}$$

where α is a phenomenological parameter embedding the dependency of the shear viscosity on the orientation. This formulation gives rise to directional dependency of the shear viscosity. Indeed, Eq. (4) in index notation reads

$$\sigma_{ij} = \left[p - \lambda D_{kk}\right] \delta_{ij} - 2H_{ijkl} D'_{kl}, \tag{5}$$

where we have introduced the fourth order shear viscosity tensor as

$$H_{ijkl} = \eta \left[\delta_{ik}\delta_{jl} - 3\alpha \left(\delta_{ik}A'_{lj} + A'_{ik}\delta_{jl} - 2/3 A'_{kl}\delta_{ij}\right)\right]. \tag{6}$$

Scalar shear viscosity emerges only for $\mathbf{A}' = \mathbf{0}$, that is in the absence of alignment.

The parameter α cannot take any value, given that dissipation considerations [22] require that

$$\boldsymbol{\sigma} : \mathbf{D} \leq 0 \Rightarrow \alpha \leq 1. \tag{7}$$

To further understand the role of the phenomenological parameter α, consider unidirectional, homogeneous shear flows (Fig. 1b), in which convex grains are completely aligned with the streamlines, which is physically admissible only for grains of extreme aspect ratios, $|r_g| \to 1$. In this configuration, the shear stress, τ, takes the simple form

$$\tau = \eta\dot{\gamma}(1 - \alpha), \tag{8}$$

where $\dot{\gamma}$ is the shear rate. If perfectly aligned in the flow direction, the convex particles can only slide over each other, so that the macroscopic friction, that is the ratio of the shear stress to the pressure, must equal the coefficient of sliding friction, μ, of the single grain,

$$\tau/p = \eta\dot{\gamma}/p(1 - \alpha) = \mu. \tag{9}$$

Equation (9) suggests that α must depend on the friction coefficient μ and be $\alpha = 1$ for frictionless, convex grains. For more complicated, non-convex shapes, such as polymers composed of (partially overlapped) spheres [17], α should depend also on other surface features.

Given that the orientational tensor is an additional state variable, we need to phrase a balance equation for $\mathbf{A}$ that must depend on the other hydrodynamic fields and the particle properties. The balance proposed in [23] explicitly included a term that induces particle alignment in the flow direction and a relaxation term towards an isotropic, randomly oriented state. The authors took the inverse shear rate as the time scale associated with the relaxation process. If the relaxation is due to the randomizing effect of collisions, and in the context of kinetic theory, a more physically-grounded time scale for the relaxation term should be, instead, the inverse of the collision frequency, $T^{1/2}d_v^{-1}$, so that the evolution law for the orientational tensor reads

$$\mathring{\mathbf{A}} = \phi \left[\mathbf{AD} + \mathbf{DA} - 2(\,\mathbf{A} : \mathbf{D}\,)\mathbf{A}\right] - \psi T^{1/2} d_v^{-1} \mathbf{A}', \tag{10}$$

where $\mathring{\mathbf{A}} = \dot{\mathbf{A}} - \mathbf{WA} + \mathbf{AW}$ is the objective Jaumann derivative, and $\dot{\mathbf{A}}$ is the material time derivative of the orientational tensor, respectively. The two dimensionless model parameters are ϕ, which represents the tendency to align with the flow, and ψ, which is the compliance to relaxation towards misalignment due to collisions.

For Eq. (10) to be a meaningful representation of the physics, the phenomenological parameters should be independent of the quantities $\{\mathbf{L}, T\}$ that explicitly appear in the equation. Moreover, ϕ should be a function of the aspect ratio, $\phi(r_g)$, and independent of the solid volume fraction, since it accounts for interaction with the flow. We emphasize that, for prolate grains, $r_g > 0$, the orientation, $(\mathbf{k} \otimes \mathbf{k})$, is defined along their larger dimension, while for oblate grains, $r_g < 0$, it is defined along their smaller dimension. The parameter ϕ, therefore, should take positive and negative values for prolate and oblate grains, respectively, reflecting the tendency of the grain largest dimension to align with the flow. Then, we expect $\phi(r_g)$ to be approximately a monotonic and odd function, with $\phi(0) \approx 0$, and the limits $\phi \to \pm 1$ for $r_g \to \pm 1$, respectively, for perfect convection with the flow.

The relaxation parameter ψ, associated with the response to collision may in general depend on the aspect ratio, the solid volume fraction and the coefficients of normal restitution and sliding friction $\psi(r_g, \nu, e_n, \mu)$. On physical ground, we expect $\psi \geq 0$, and be approximately an even function of the aspect ratio, monotonically decreasing with $|r_g|$, with the limit $\psi \to 0$ for $|r_g| \to 1$.

We also expect ψ to be a monotonically decreasing function of the solid volume fraction, reflecting the increase in resistance to misalignment when the grains are densely packed.

The three phenomenological parameters $\{\alpha, \phi, \psi\}$ are determined by comparison with discrete element simulations. The expectations discussed above on their functional forms are based on their roles in the proposed equations for the stress Eq. (4) and the orientation, Eq. (10), and serves as validation (or invalidation) of their ability to accurately predict the rheological response. We employ literature [5, 6] measurements of stresses, granular temperature and alignment performed on discrete element simulations of steady, homogeneous, shearing flows of true, frictionless cylinders covering a large range of aspect ratios, $r_g = \{-0.8 \text{ to } +0.8\}$, volume fractions, $\nu = \{0.2 \text{ to } 0.6\}$, and coefficients of normal restitution $e_n = \{0.7, 0.95\}$. The flow configuration is reported in Fig. 1(b), with the associated frame of reference, where x, y and z represents the flow, shear and vorticity directions, respectively. Figure 1(b) also shows the director $\mathbf{u}$ (the vector associated with preferential alignment) and the angle θ that it forms with respect to the flow x-direction. Given that our evolution law for the orientational tensor Eq. (10) is independent of the stress tensor, the parameters ϕ and ψ can be determined independently of α.

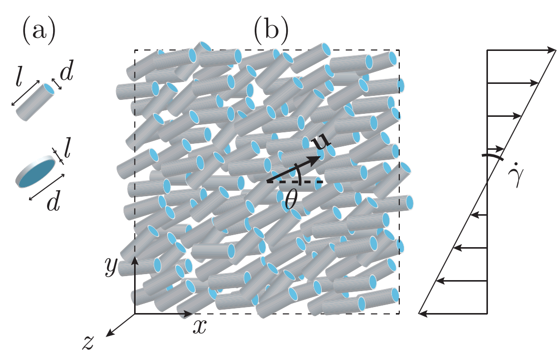

FIG. 1. (a) Examples of prolate and oblate cylinders. (b) Homogeneous shear flow configuration, with the associated frame of reference and the uniform shear rate $\dot{\gamma}$. Also shown are the director $\mathbf{u}$ and its angle θ with respect to the flow direction.

First, we use a least square fitting method to determine the parameters ϕ and ψ in order to reproduce the measurements in the simulations of the largest eigenvalue (the alignment measure S) and the associated eigenvector (in particular, its angle θ with respect to the flow direction) of the orientational tensor $\mathbf{A}$. In the balance Eq. (10), we employ the granular temperature measured in the discrete simulations. We repeat the procedure for all available values of aspect ratio, volume fraction and coefficient of restitution. Figure 2 depicts the values of the orientational parameters ϕ and ψ, and the corresponding values of S and θ, as functions of the solid volume fraction for various aspect ratios.

Figure 2(a) indicates that, for $r_g = 0$, the tendency to align with the flow vanishes, as $\phi \approx 0$, and the only steady-state solution of Eq. (10) is no alignment, $\mathbf{A}' = \mathbf{0}$, independently of the value of ψ. Additionally, the figure confirms that $\phi(r_g)$ is approximately an odd function of r_g, roughly independent of the solid volume fraction. The latter statement is especially true if we disregard the results for $\nu \leq 0.3$, where there is no significant alignment and the obtained values of the model parameters are less reliable. Figure 2(b) shows that ψ is a monotonically decreasing function of ν and $|r_g|$, as expected. We have checked that ϕ and ψ do not depend on the coefficient of restitution. Tentative interpolating formulas for the orientational parameters ϕ and ψ are reported in the caption of Fig 2. The dependency on the aspect ratio obtained here is similar to [23], where polymers formed by conglomerate of spheres rather than cylinders were considered. However, here we have additional dependency on the solid volume fraction. As already noticed [5], non-spherical granular particles exhibits a transition from isotropic (random orientation) to nematic (preferential orientation) phase in response to change in solid volume fraction, as demonstrated by the increase in the alignment measure S with ν. However, in homogeneous shearing flows, the granular temperature is not independent of the solid volume fraction [4]: it would be interesting to investigate other configurations in which T and ν can vary independently of each other to check if the phase transition can also be induced by suppressing the particle agitation.

We emphasize that the orientational parameters represent the interaction of the grains with the surrounding, and as such they should be sensitive to the shape of the grains, not only to their aspect ratio. We therefore expect slight, quantitative, but not qualitative, differences in the dependence of ϕ and ψ on the aspect ratio and the solid volume fraction if, e.g., sphero-cylinders [24] or polymers [23] are considered, rather than true cylinders. The dependence of the orientational parameters on the coefficient of sliding friction remains to be determined.

Once the orientational parameters ϕ and ψ are known, Eq. (10) can be solved to determine all elements of the orientational tensor $\mathbf{A}$ and, then, via Eq. (4), the stress tensor. In the homogeneous shearing flow configuration of Fig. 1(b), where the only non-zero elements of the rate of deformation, $\mathbf{D}$, are $D_{xy} = D_{yx} = \dot{\gamma}/2$, the shear stress, $\tau = -\sigma_{xy}$, reads:

$$\tau = \eta \left[1 - 3\alpha \left(A'_{xx} + A'_{yy}\right)\right] \dot{\gamma}. \tag{11}$$

In the case of frictionless cylinders, $\alpha = 1$, as already mentioned. In Eq. (11), η is evaluated with Eq. (3), using the same coefficient of restitution e_n of the simulations and the critical volume fraction $\nu_c = 0.67$, as appropriated for frictionless cylinders [4] (we neglect any small dependence of the critical volume fraction on the aspect ratio).

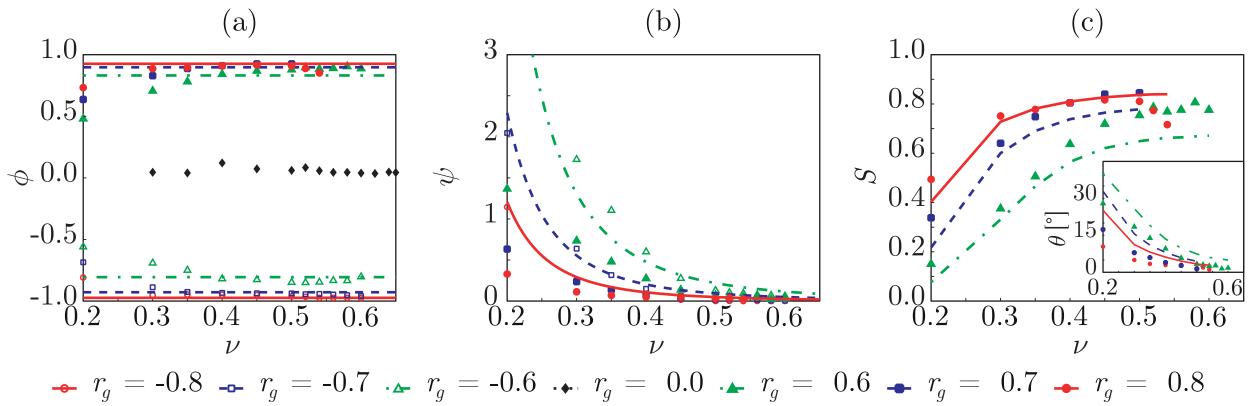

FIG. 2. Fitted values (symbols) of the orientational parameters (a) ϕ and (b) ψ as functions of the solid volume fraction for different aspect ratios of frictionless cylinders (only values for $e_n = 0.95$ are shown). The lines represent the interpolating functions $\phi(r_g) = a_1 \tan^{-1}(a_2|r_g|^{a_3} + a_4)$ and $\psi(\nu, r_g) = b_1\nu^{b_2}(1 - |r_g|)^{b_3}$, where: $\{a_i\} = \{0.75, 4.0, 1.4, 0.05\}$, for $r_g \geq 0$; $\{a_i\} = \{0.75, -6.8, 2.5, 0.05\}$, for $r_g \leq 0$; and $\{b_i\} = \{0.2, -3.5, 2.55\}$. Corresponding values of (c) the alignment measure S and (inset) the angle θ between the director and the flow as functions of the solid volume fraction measured in the discrete simulations (symbols) and obtained by solving the balance Eq. (10) (lines) in the case of prolate cylinders.

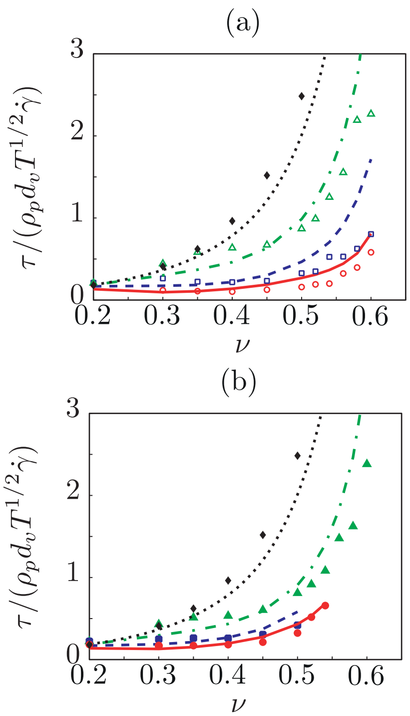

FIG. 3. Predicted (lines) and measured in discrete simulations (symbols) dimensionless particle viscosity as a function of the solid volume fraction at different values of the aspect ratio of (a) oblate and (b) prolate frictionless cylinders ($e_n = 0.95$). Same legend as in Fig. 2.

Figure 3 depicts the comparison between the dimensionless particle viscosity, $\tau/\left(\rho_p d_v T^{1/2}\dot{\gamma}\right)$, predicted by our model (Eq. 11) and that measured in the discrete simulations of homogeneous, shearing flows of frictionless cylinders at $e_n = 0.95$ [5]. The significant reduction in the shear viscosity associated with the preferential orientation of the grains, signature of a phase transition from an isotropic to a nematic phase, is indeed well captured by simply including a linear dependency on the orientational tensor in the constitutive law for the stress tensor (Eq. (4)). A similar satisfactory agreement, not shown here for brevity, is obtained also for $e_n = 0.7$.

In summary, we have proposed a generalized granular kinetic theory for uniaxial, non-spherical grains, that includes a linear dependency on the orientational tensor into the constitutive law for the stresses, and a balance law for the orientational tensor itself, in which a key role is played by the randomizing effect of collisions. The generalized model has only three additional phenomenological parameters that have clear physical meaning, and can, therefore, be uniquely determined from simple experiments or discrete numerical simulations. One of them must be equal to one in the case of frictionless, convex grains; its value and the values of the other parameters for frictional grains remain an open question. We emphasize that, while the parameters have been determined in steady, homogeneous shearing flows, the model is general and can be potentially applied to other flow configurations, e.g., inhomogeneous, boundary-value problems, in which boundary conditions for the orientational tensor must be provided [3]. In this work, we have not addressed how the preferential alignment of non-spherical grains affect the balance of fluctuation energy for the particles, which determines the granular temperature. Existing works on the subject have either focused on non-sperical particles in the absence of alignment [9, 10], or have included only the role of the alignment measure S [6]. Including the full orientational tensor in the fluctuation energy balance is a task for the future. Finally, linear kinetic theories, such as the one that we have generalized here, are unable to capture the normal stress differences typical of granular flows [15]. Hence, it would be tantalizing to include a linear dependency on the orientatonal tensor in a non-linear kinetic theory [20, 26] to assess the coupled role of alignment and anisotropic fluctuations on the normal stresses.

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[1] $g_0 = \frac{2-\nu}{2(1-\nu)^3}$, if $\nu \leq 0.4$; and $g_0 = \left[1 - \left(\frac{\nu-0.4}{\nu_c-0.4}\right)^2\right] \frac{2-\nu}{2(1-\nu)^3} + \left(\frac{\nu-0.4}{\nu_c-0.4}\right) \frac{2}{\nu_c-\nu}$, if $\nu \geq 0.4$, after [31].

[2] $J = (1 + e_n)/2 + (\pi/32)[5 + 2(1 + e_n)(3e_n - 1)\nu g_0][5 + 4(1 + e_n)\nu g_0]/[(24 - 6(1 - e_n)^2 - 5(1 - e_n^2))\nu^2 g_0^2]$, after, e.g., [21].

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