Letter

Simple generalization of kinetic theory for granular flows of nonspherical, oriented particles

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We generalize kinetic theory of inelastic spheres to uniaxial, nonspherical grains by including the orientational tensor as a state variable. The theory has three phenomenological parameters, with one parameter to account for the dependency of the stresses on the orientation, which is exactly one for frictionless cylinders, and the other two parameters to predict the orientational tensor. 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 a significant reduction in the viscosity in response to alignment measured in discrete simulations of homogeneous shear flows of prolate and oblate frictionless cylinders.

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Kinetic theory of granular gases [1,2] 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 [3,4]. 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 nonspherical 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 [5–8]. 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 a subject of intense research activity on molecular liquid crystals—random assemblies of nonspherical molecules that can show preferential orientation in response to change in temperature, concentration, and/or when subjected to external fields [9–13]. Granular, nonspherical 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

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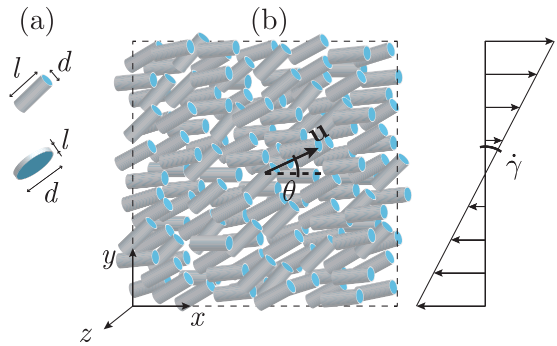

FIG. 1. (a) Examples of prolate and oblate cylinders. (b) Homogeneous shear flow configuration, with the associated frame of reference and the uniform shear rate $\dot{\gamma}$. Also shown are the director $\mathbf{u}$ and its angle θ with respect to the flow direction.

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 a 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 ith 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, $0 \leqslant S \leqslant 1$, 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 [14]. The measure S vanishes in the absence of alignment ($\mathbf{A}' = \mathbf{0}$) and equals 1 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. The 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 [1]:

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

where p is the hydrostatic pressure, and 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 [16] of the coefficient of normal restitution, e_n (the negative of the ratio of postcollisional to precollisional, normal relative velocity between colliding grains, here taken to be a constant), and the solid volume fraction [17], and g_0 is the radial distribution function at contact [18], which is also a known function [19] 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 [20]. 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 [21,22]. Expressions for the pressure and the volumetric viscosity can also be found in [1].

For granular materials composed of identical, hard, uniaxial, nonspherical grains, we generalize Eq. (2) to include a linear dependency on the orientational tensor into the deviatoric part of the stress tensor [23],

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

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

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

where we have introduced the fourth-order shear viscosity tensor as

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

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 [23] require that

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

To further understand the role of the phenomenological parameter α, consider unidirectional, homogeneous shear flows [Fig. 1(b)] 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, nonconvex shapes, such as polymers composed of (partially overlapped) spheres [24], α should depend also on other surface features.

Given that the orientational tensor is an additional state variable, we need to phrase a balance law for $\mathbf{A}$ that must depend on the other hydrodynamic fields and the particle properties. The balance proposed in [25] 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 timescale associated with the relaxation process. If the relaxation is due to the randomizing effect of collisions, in the context of kinetic theory, a more physically grounded timescale 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

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

where $\mathring{\mathbf{A}} = \dot{\mathbf{A}} - \mathbf{W}\mathbf{A} + \mathbf{A}\mathbf{W}$ 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. We then 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 grounds we expect $\psi \geqslant 0$ and to monotonically decrease 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 tensor, 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 represent 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.

The two parameters $\{\phi, \psi\}$ are uniquely determined by requiring that 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 obtained by solving Eq. (10) at steady state, $\dot{\mathbf{A}} = \mathbf{0}$, give exactly the two measured properties $\{S, \theta\}$ reported in [5]. In the balance 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 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 $\nu \leqslant 0.3$, 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 simple 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 [25], where polymers formed by conglomerates of spheres rather than cylinders were considered. However, here we have additional dependency on the solid volume fraction. When we use these simple interpolating functions to solve for Eq. (10), we obtain the behavior of S and θ with the solid volume fraction and the aspect ratio depicted in Fig 2(c). The agreement is relatively good, and, potentially, it could be improved with better interpolation functions that perhaps distinguish between prolate and oblate grains, especially in the determination of ψ. Nevertheless, we find

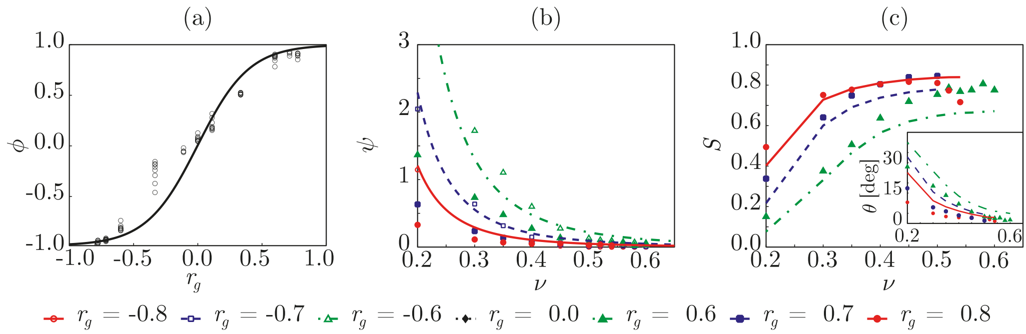

FIG. 2. Fitted values (symbols) of the orientational parameters (a) ϕ as a function of r_g (all solid volume fractions) and (b) ψ as a function of the solid volume fraction for different aspect ratios of frictionless cylinders (only values for $e_n = 0.95$ are shown). The lines represent the interpolating functions $\phi(r_g) = 2/[1 + \exp(-a\, r_g)] - 1$ and $\psi(\nu, r_g) = b_1 \nu^{b_2}(1 - |r_g|)^{b_3}$, where $a = 5$ 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) with the interpolating functions in the case of prolate cylinders.

these approximations to be satisfactory for our purpose, considering that they are compared with measured data from discrete simulations which inevitably contain errors. As already noticed [5], nonspherical granular particles exhibit 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 [26]: 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., spherocylinders [7] or polymers [25] 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 **A** and then, via Eq. (4), the stress tensor. In the homogeneous shearing flow configuration of Fig. 1(b), where the only nonzero elements of the rate of deformation, **D**, are $D_{xy} = D_{yx} = \dot{\gamma}/2$, the shear stress, $\tau = -\sigma_{xy}$, reads

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

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 [26] (we neglect any small dependence of the critical volume fraction on the aspect ratio).

Figure 3 depicts the comparison between the dimensionless particle viscosity, $\tau/(\rho_p d_v T^{1/2}\dot{\gamma})$, 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 equation for the stress tensor [Eq. (4)]. A similar satisfactory agreement, not shown here for brevity, is obtained also for $e_n = 0.7$. While the viscosity in prolate cylinders is very well captured, even at the largest values of the solid volume

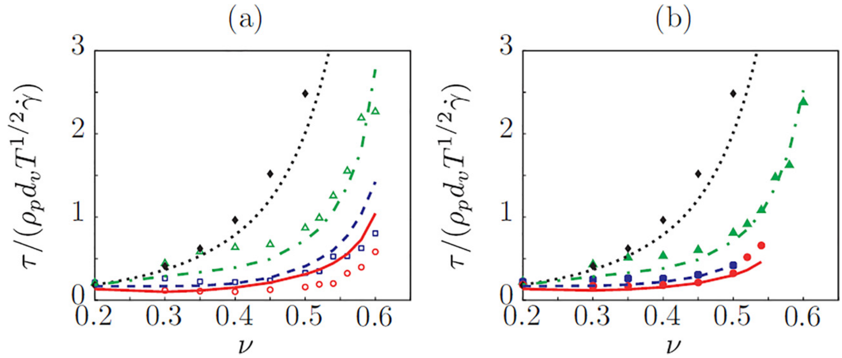

FIG. 3. Predicted (lines) and measured in discrete simulations (symbols) dimensionless particle viscosity as a function of the solid volume fraction at different values of the aspect ratio of (a) oblate and (b) prolate frictionless cylinders ($e_n = 0.95$). Same legend as in Fig. 2.

fraction [Fig. 3(b)], the agreement is less impressive for oblate cylinders [Fig. 3(a)]. Once again, we could have improved our findings by introducing asymmetries in the dependence of ϕ and ψ on the aspect ratio, and, perhaps, being fastidious on the variation of ν_c with r_g. However, these would be second-order refinements, while we claim that our model captures the essential physics.

In summary, we have proposed a generalized granular kinetic theory for uniaxial, nonspherical grains that includes a linear dependency on the orientational tensor into the constitutive equation 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 1 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 [27]. In this work we have not addressed how the preferential alignment of nonspherical grains affects the balance of fluctuation energy for the particles, which determines the granular temperature. Existing works on the subject have either focused on nonspherical particles in the absence of alignment [28,29] 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 orientational tensor in a nonlinear kinetic theory [30,31] to assess the coupled role of alignment and anisotropic fluctuations on the normal stresses.

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