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On the continuum modeling of dense granular flow in high shear granulation

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ABSTRACT

This article addresses the subject of continuum modeling of dense granular flows with an application in high shear granulation. The possible use of continuum models and their ability to reproduce correct dynamics of such flows has been a subject of debate for a long time in the literature, and no consensus has been achieved so far. In this paper, we examine and compare two ways for making it possible to study dense granular flows in a continuum framework: the one that considers the stress tensor of a particulate phase as a sum of frictional and kinetic-collisional terms and the one that is based on modification of transport coefficients of the kinetic theory of granular flow. The latter framework is based on an analogy with molecular systems and how they behave at the phase transition from a liquid to a crystalline state. We show here that the formulation proposed in this work is able to correctly capture the phase transition and coexistence of solid-like and fluid-like phases in dense granular flows. This is in contrast to the model with added friction where the stress-strain dependence is shown to give a qualitatively different behavior compared to experimental data.

1. Introduction and background

Granular flows are present in many large-scale industrial processes where particles and powders are transported or mixed. The modeling approaches for resolving the behavior of particles in these systems can be divided into two categories: discrete element modeling (DEM), where the forces acting on each particle are calculated in order to give its individual trajectory, or a continuum approach, in which the particles are treated as a continuous phase. When one deals with a large-scale process and thereby with an enormous amount of small particles, the use of continuum models is advocated. The computational cost of using DEM tends to become unfeasible for simulating the amount of particles present in an industrial system. However, the use of a continuum approach in such situations is not always straightforward and has been a subject of debate in literature over the years. The continuum framework implies averaging over a number of particles and thus avoids resolving individual particle motion [1]. Strictly speaking, such an approach is applicable in systems where there is a clear separation between the microscopic (i.e., related to the mean free path or mean collisional time) and macroscopic time and length scales [2]. It can be shown [3] that, for granular flows, this separation of scales is only present for systems where the particle–particle collisions are elastic or nearly elastic. Different and sometimes opposing points of view are present regarding the possibility to extend the continuum framework to larger degrees of inelasticity. The models developed by Garzo and Dufty [4] and Sela and Goldhirsch [2] are two examples of models that successfully capture features of flow of inelastic particles in a continuum framework, while, for example, Campbell [5] argues against their use due to the violations made in the averaging process. In this study, we restrict ourselves to the flow of nearly elastic particles. We focus not only on the use of continuum models for treating dense granular flow but also on the coexistence of dense and relatively dilute regions and on capturing the transition between them. High shear granulation (HSG) indeed represents an example of a process where both such regions are present in a large-scale unit. HSG is a unit operation in the process of manufacturing tablets and pills. It serves to mix and coalesce solid ingredients in powder form. The ability to model the flow conditions in industrial-scale HSG equipment has been deemed crucial for further development of predictive models for the granule properties [6,7].

As indicated above, in a typical HSG equipment there is coexistence of relatively dilute (solid volume fractions ranging from 0 to 0.5) and very dense regions (ranging from a volume fraction of 0.5 to the maximum packing of the material) [8,9]. The flow situation in the former region is most often described by the rapid flow theory, whereas in the latter, the quasi-static flow regime is assumed. In the quasi-static regime, there is little particle motion and in a continuum framework, the behavior is governed by the pressure on the closely packed granules and possible frictional sliding [10,11]. On the other hand, in the rapid regime, the behavior is predominantly governed by binary collisions and particle translation [1,3,13,14]. The behavior is said to be gas-like since it in many ways resembles that of molecular ideal gases [15]. In the

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transition regime, there is a liquid-like state in which a collective behavior governs the main motion of the particles, but the particles are still free to have individual velocity fluctuations. The transition between these regions is a key feature to capture in order to correctly describe the flow in HSG equipment. In literature, there is no consensus on a model that can handle this transition or the coexistence of the mentioned regions. To accommodate such a behavior in a continuum framework, three possible directions can be taken: (i) to extend quasi-static descriptions based on friction and elasticity to the relatively dilute high-velocity state; (ii) to start from a rapid, high velocity, collisional regime and modify it to ensure that high-volume-fraction effects are taken into account; or (iii) to take on a rheological approach to treat the liquid transition region combining it with models for both the quasi-static and rapid regions. An example of the last mentioned approach is the model developed by Jop et al. [16] and treating the granular phase as a visco-plastic fluid. This approach focuses on the transition regime capturing the liquid–solid transition with a pressure-dependent yield stress determined for individual particle types and sizes from a set of flow experiments. The results show good potential, but the model is not capable of treating the rapid regime [8]. In Khalilitehrani et al. [17], the framework was extended and combined with a rapid regime, kinetic theory of granular flow (KTGF), model with a transition criterion based on a regime determining inertial number.

The models with their starting point in the quasi-static regime use concepts from solid mechanics, such as yield criteria and flow rules [10]. The solid phase stress is shear-rate independent [18] and some examples of models belonging to this group are the papers by Shaeffer [10] and Johnson and Jackson [11]. These models use the Mohr–Coulomb type of expressions to treat the stress transmissions under shear. The models are then extended for the use in regime transition systems by addition of a dilute phase model. This somewhat improvised approach treats the liquid regime as a linear combination of the two bordering states [11]. In the regions where the yield criteria are not fulfilled, the stress transmission becomes direct, like in a solid. This leads to a non-local strain dependence of the stresses, in which the overall stress tensor is expressed as a sum of a viscous stress and a non-local component. There are examples of non-local solid phase models, i.e., Mills et al. [19] and Pouliquene and Forterre [20], where long range stress transmission is accounted for by integrating the stresses over the estimated correlation length, obtained under different conditions. This long distance transmission of stresses is present also in the liquid state [21,22] and is responsible for the collective behavior of particles in this regime. However, for the use in large-scale equipment, it would be computationally preferable to be able to use a local model that can still capture these features.

Bagnold (1954) [12] was probably one of the first who looked at the continuum behavior of granular gas systems, and the study resulted with a famous quadratic dependence of the stresses on the shear rate. This behavior is in accordance with the later developed models based on KTGF [14,13]. KTGF is based on a series expansion solution to a number of statistical moments of the Boltzmann equation. For dilute systems of elastic particles, there are a number of solutions using an expansion around the equilibrium state, represented by a Gaussian particle state distribution function [1,23,24]. To be able to use the theory for dense systems, Santos et al. [25], Dufty et al. [26] and Garzo and Dufty [4] used a different equilibrium solution shown to correctly represent the particle state distribution for all volume fractions, even to the maximum packing limit of the system. The approach is termed the revised Enskog theory (RET) [27] and has shown promising results. The series expansion can be performed to different orders, where the first order (giving the Navier–Stokes equations) is typically used. Sela and Goldhirsh [2] have shown that retaining also the second order terms (the Burnett order) gives results that can predict the collective behavior of particles at higher volume fractions. However, the Burnett order equations are ill-posed [2], and hence, the solution of the hydrodynamic expressions becomes not so straightforward. A different strategy for capturing the collective behavior of particles in a dense granular flow has been identified when the rate of divergence (in volume fraction) of the shear viscosity is increased in relation to the divergence rates of the transport coefficients concerning the random velocity fluctuations of the particles [28,29]. Such a behavior of the shear viscosity results in a more collective mean motion of the particles as the packing approaches that of the random close packing. At the same time, it is assumed that the velocity fluctuations are not affected by this limit. The quantification of the divergence rate is based on experiments and detailed DEM simulations [30]. By introducing this observation into the KTGF model, we believe that we can capture the collective behavior in the transition regime. Note that this type of viscosity divergence can also be seen in molecular systems in the crystallization limit [30]. The approach hence shows potential to describe the full set of regimes, from quasi-static to rapid flow ones.

In the field of high shear granulation, continuum models were used by Darelius et al. [31], Ng et al. [9] and Abrahamsson et al. [32]. All these studies used a KTGF model with an added friction model (KTGF + Friction) in the dense regions. Discrepancies were observed in the dense regions where the predicted viscosity was found to be too small. A different approach was taken in a study of a disc impeller granulator by Khalilitehrani et al. [8], in which the authors looked at the flow that is purely in the transition regime. Khalilitehrani et al. [8] used the rheology model, developed by Jop et al. [16], that treats the granular phase as an incompressible visco-plastic fluid. The obtained results showed good potential, but the constant volume fraction assumption was found to lead to erroneous predictions even for the simple system of a disc impeller. Benefiting from a combination of rheology and KTGF models, a further attempt was made to simulate a disc impeller system [17]. The results showed improvements in being able to resolve volume fraction profiles and granular temperatures in the agitated regions. The described modeling approach is promising but uses different models for different regimes. However, the use of a physically based switching criterion is a great improvement as compared to the additive method used in the KTGF + Friction model.

This article aims to investigate, in detail and within a single framework, the potential of using a modified approach, here termed the viscosity divergence model, to capture the coexistence of different regimes of granular flow and transitions between them. Here, the application of interest is HSG, but the results are general for all applications in which there exists more than a single regime of granular flow. In this paper, we will compare the proposed approach with the KTGF with added friction [11] and, as a reference, with the case when the "pure" KTGF (using the Enskog theory) is used [13,14]. The study will be done for a Couette shear cell. This configuration allows for relatively fast calculations and a straightforward analysis, while retaining the physics of a sheared granular flow. Furthermore, there are available experimental data for the purpose of evaluating both the qualitative and quantitative behaviors of the different models.

2. Theory and model description

The models compared will be the KTGF model by Lun et al. [14] and Gidaspow and Ding [13], the KTGF model with an added frictional model by Shaeffer [10] and Johnson and Jackson [11] and the viscosity divergence model originally proposed by Bocquet et al. [28]. In this section, the underlying assumptions and brief descriptions of the derivations of all the mentioned models will be presented.

The viscosity divergence model is in its foundation a KTGF model. A brief recovery of the derivation of the KTGF model will therefore be given here, focusing on the assumptions made regarding the particle and flow properties. This is followed by a short description of the frictional model that is added to the KTGF in the "KTGF + Friction" approach. At the end of this section, the viscosity divergence model is described in detail.