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On continuum modelling of dense inelastic granular flows of relevance for high shear granulation

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ABSTRACT

This article investigates a number of possible formulations of a continuum description for modelling dense inelastic granular flows. The revised Enskog theory (RET) for expressing the granular temperature and formulation of transport coefficients has been used within the continuum framework. The framework assumes particles as inelastic spheres and can describe a granular system at a wide range of volume fractions. The transport coefficients depend on the volume fraction through a modified expression for the radial distribution function. The proposed radial distribution function is based on previous studies on the behaviour of the shear viscosity in which an earlier divergence of the latter compared to the other transport coefficients has been demonstrated for sheared dense granular systems. Our results show that the newly developed radial distribution function maintains the ability of RET to predict the occurrence of instabilities in a homogeneous cooling granular gas. The introduced function also improves predictions for the velocity and volume fraction profiles in a Couette cell dense shear flow. Thus the proposed expression shows promising features in terms of improving predictions for volume fractions relevant in high shear granulators. We have also observed that a different expression may be needed for the densest regions.

1. Introduction

Dense flows of inelastic particles are common both in nature, for example landslides and avalanches, [1] and in industrial applications, either for material transport as in conveyers and hoppers [2], or as a part of the product refining in terms of fluidized beds [3] or granulation equipment [4]. It is generally agreed that reliable models for predictive modelling of particulate processes are still largely missing.

One example of a production step that involves dense flow of inelastic particles is High Shear Granulation (HSG), which is an important unit operation with many fields of use. An important application of this technology is in the pharmaceutical industry where it is a common unit operation for production of tablets. A reliable flow model would be of great relevance for both describing the existing units and designing new ones. In general, two modelling approaches are commonly used; Discrete Element Modelling (DEM) and continuum modelling. Gantt et al. [5] used DEM to look at collision rates of particles in a small-scale HSG equipment. The downside of DEM is its high computational cost of resolving all collisions and all particle trajectories, which makes it unfeasible to model production-scale equipment. To be able to model large scale units, the use of continuum models is preferred. Darelius et al. [6] and Ng et al. [7] were the first to use the continuum approach on the HSG equipment. The same approach was further used in Abrahamsson et al. [8]. These studies used the kinetic theory of granular flow (KTGF), as formulated by Lun et al. [9] with the added frictional model developed by Shaefer [10] and Johnson and Jackson [11]. The results showed not only a certain degree of agreement with experimental data, but also discrepancies in the dense particle regions where the frictional model has been made active.

To improve model description of the behaviour in the dense particle regime, the studies by Khaliliteherani et al. [12,13] used a Herschel–Bulkley liquid-like rheology model, which applies experimentally found parameters from a chute flow, to describe the stress–strain relation of the material. The model assumes a constant volume fraction of solids and a local stress–strain relation, while the parameters are based on chute flow experiments. However, it does not invoke any other restrictions on the flow or particles, such as the degree of elasticity of collisions or the type of particle interactions (binary or multiple). Khalilitherani et al. [13] combined the rheology approach with the KTGF to describe all regions of flow in HSG equipment. This approach certainly shows potential, but the KTGF model used does not perform adequately in dense regions [13]. The Lun et al. [9] model is based on the assumption of a dilute particle system and with nearly elastic collisions. Abrahamsson et al. [14] investigated other options for the volume fraction dependence of the shear viscosity in a dense sheared particle system. That study is based on the work of Bocquet et al. [15], which examines the volume fraction dependence of the shear viscosity and especially its behaviour in regions where particles are packed close to maximum packing. The shear viscosity diverges at a significantly

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higher rate than do the other transport coefficients. The latter coefficients still use the volume fraction dependencies from the KTGF theory devised by Lun et al. [9]. The approach that takes into account the described behaviour of the shear viscosity will in this article be referred to as the "viscosity divergence model", emphasizing the modification that it introduces as compared to the KTGF. Abrahamsson et al. [14] showed that this modelling framework was able to capture the experimental stress–strain behaviour in the transition from a collisional to frictional behaviour for nearly elastic particles.

On the other hand, it is evident that, in order to treat realistic systems, there is a need for models that can handle inelastic particles at medium to high solid volume fractions. This study represents a step in that effort. The treatment of inelasticity within the framework of KTGF models has been addressed in several different ways. Saha and Alam [16] used the Burnett and super Burnett equations [17] and showed that the preservation of these terms in the Enskog solution [18] is a necessity for inelastic systems to predict normal stress differences and anisotropies in velocity fluctuations. The same observation was also made previously in [19] which recognized the non-Newtonian nature of the granular fluid, as given by the anisotropic stress tensor. In contrast, Montanero et al. [20] have shown that even the Navier–Stokes order transport coefficients still can resolve many features of flows involving inelastic smooth spheres. These features include the change in the shear rate dependence of the viscosity from a negative dependence, shear thinning, to a positive one, shear thickening, as the volume fraction increases [21]. Mitrano et al. [22] showed that the Navier–Stokes order equations could resolve the instability of a homogeneous cooling granular gas using the Revised Enskog Theory (RET). There are stability benefits of staying with the Navier–Stokes order equations. Sela and Goldhirsh [17] state that the set of Burnett-order equations derived in their study are ill posed, and that for implementation in an industrial system, which is far from equilibrium, stability of a solution is of great importance.

The goal of the present study is to investigate and develop expressions for the Navier–Stokes order transport coefficients for dense inelastic granular flows. Our expression uses features from RET [23] while making use of the volume fraction dependence of the shear viscosity from the viscosity divergence framework [15]. The latter dependence was proven beneficial in a previous study by Abrahamsson et al. [14]. The framework will be compared to the following continuum representations of dense granular flows: the one by Garzo et al., here termed the revised Enskog theory (RET), the Bocquet et.al. model, here termed the Visc.div. model and, as a benchmark, the Lun et al. model [9], here termed the Enskog model. The models will be evaluated in a Couette shear cell geometry and in a 3D uniformly cooling granular gas. The former setup has been chosen in order to test the models on a non-equilibrium, dense sheared system, whereas the second one will serve as to test the validity of the Navier–Stokes order models for cases in which dissipative collisions lead to pronounced instabilities in the form of particle clusters. Our intention here is to assess whether the mentioned models can be applicable for modelling dense inelastic granular flows in a realistic unit from process industry, such as, for example, a high shear granulator. Note that in its current form, the models do not include cohesion between particles. This effect could, however, be added in the way it was done by, for example, van Wachem and Sasic [33].

2. Model description and theory

In this section we will go through theoretical backgrounds of the models for dense, inelastic granular flows used in the paper. Our aim is to put forward their respective benefits and drawbacks. We start with the revised Enskog theory and continue with the viscosity divergence model.

2.1. The revised Enskog theory

The KTGF models based on the Enskog theory [18], such as Lun et.al. [9], are built on the assumptions of a dilute system of elastic or nearly elastic particles. This is partially due to the equilibrium description used as the starting point for the perturbative solution. In the Enskog solution the particle properties are described by the probability density function, PDF, which describes the likelihood of finding particles within a certain property interval. The PDF in the Enskog solution is a Gaussian distribution which is valid only for a dilute elastic particle system.

The revised Enskog theory (RET) was developed by van Beijeren and Ernst [24]. The authors developed equations for the equilibrium description of the particle property distribution, f, in systems of smooth hard spheres. This equation is similar to the Boltzmann equation; however, it uses a fractional dependence of f on the field variables (to be described later). Such a formulation leads to a correct description of the system at equilibrium at a wide range of volume fractions, from dense to dilute. Note that a system is said to be at equilibrium if the gradients of relevant hydrodynamic fields do not change at distances of a few mean free paths of the particles. It is also worth mentioning that the collisional contribution to the momentum transfer, defined as the collision integral in the Enskog solution, is still based on the assumptions of non-correlated particle motion and binary and instantaneous particle–particle interactions. In addition, there are no effects of friction, and, consequently, no effects of rotational momentum and dissipation via frictional sliding. The hydrodynamic models based on RET, in which the first three statistical moments of $f(r_1, v_1, t)$ are derived, have been presented by Dufty et al. [25]. These models for transport coefficients show good agreement with both experimental and DEM data for equilibrium systems. These models have also been tested for non-equilibrium systems subjected to uniform shear [25] and have shown good agreement with DEM simulations. It is possible to predict the qualitative dependence of the viscosity on the shear rate, with shear thinning at low shear rates followed by shear thickening as the rate increases. This RET approach was used by Garzo and Dufty [23] and expanded to be valid for inelastic spheres. The expressions used in the present study are those derived in Garzo and Dufty [23], and for the full derivation of the equations the reader is referred to that article. The governing equations for the transport of mass momentum and granular temperature are given in Table 1 which introduces the transport coefficients that are further presented in the same table.

In the expressions in Table 1, D_t is a material derivative, U is the mean velocity field, P_{ij} is the stress tensor, ζ is the dissipation of granular temperature due to collisions, n is the number density of the particles and d is the particle diameter, m is the mass of a particle and e is the binary restitution coefficient.

The radial distribution function presented as expression T 11 in Table 1 is the Carnahan–Starling approximation which is not valid at high volume fractions [26]. The radial distribution function is a critical part of any model intended for describing a granular flow at high volume fractions. In this work, by introducing a new form of the radial distribution function, as obtained from the viscosity divergence representation, we aim to improve the predictions for dense non-equilibrium systems.

The coefficient ω is a part of the contribution to the conductivity of the granular temperature which is due to the inelasticity and is present in the equation for the granular temperature flux (q), Eq. (1).

$$q = \kappa \nabla T + \omega \nabla n \tag{1}$$

The second term on the r.h.s. of (1) is not present in typical formulations of the kinetic theory of granular flow, but is essential for systems involving inelastic particles.