# THE RELATION BETWEEN PARTICLE PROPERTIES, FLOW MICROSTRUCTURE, AND BULK POWDER FLOW

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# Contents

**Abstract**

Bulk handling, transport and processing of particulate materials such as powders and granules are integral to a wide range of industrial processes in many fields or natural, geophysical phenomena. Particulate systems are difficult to handle and display unpredictable behaviour, which represents a great challenge for both design and operation of unit operations and plants, but also for the research community of Powders and Grains. Granular materials and powders consist of discrete particles such as individual sand-grains, agglomerates (comprising of many primary particles), or bonded solid materials like sandstone, ceramics, or some metals or polymers sintered during additive manufacturing. The primary particles can be as small as nano-metres, micro-metres, or millimetres covering multiple scales in size and a variety of mechanical interaction mechanisms. Those interactions include friction and a variety of cohesive forces, which becomes more and more important the smaller the particles are. All these particle systems have a particulate, usually disordered, inhomogeneous and often anisotropic micro-structure. which is at the core of many of the challenges one faces when trying to understand powder technology and granular matter. The flow behaviour of granular materials is inherently related to the kinematic and collective behaviour of the microscopic components. On the macroscale, it is noted that the particulate nature and the salient details of the contact mechanics are not adequately captured in the constitutive relations that are needed to solve the continuum equations. The influence of the particles on the bulk behaviour has to be better understood to ultimately provide effective predictive tools for particulate flows. One promising development in bridging from micro-mechanical insights at particle- and contact-level to the next generation of superior continuum models will come from the coarse-graining methodologies. Bridging the gap between the particulate, microscopic state and the macroscopic, continuum description is one of the challenges of modern research. This work gives an overview of recent progress about the flow behaviour of collection of deformable particles and the relation with the smaller scales involved.

The key point for a better understanding of the flow behaviour is the multiscale characterisation of powders, starting from the ***microscopic*** scale of individual primary particles, to the ***macroscopic*** scale of the bulk flow, including the ***mesoscale*** that lays in between, relevant for the granular fabric and aggregates. After an introduction section, where the main differences between dry granular materials and cohesive powders are highlighted, the first part of the paper reviews both classical and state of the art experimental techniques

used in the laboratory at different scales. Section 2.1 is devoted to the characterisation of individual particle properties, as relevant for granular flows. Specifically, the focus is on mechanical properties (e.g. density using pyconometry, stiffness using atomic force microscopy or nano-indentation nano-indentation equipment, restitution coefficient - using collision test) and particle morphology (surface roughness using Atomic Force Microscopy, specific surface area using nitrogen sorption technique, roundness/sphericity using Scanning Electron Microscopy, etc.). In Section 2.2, experimental techniques developed for the analysis of the mesoscale are reviewed, typically at the size of clusters/agglomerates. First, methods used to determine compressive/tensile mechanical responses are introduced, followed by an overview of advanced techniques for the analysis of the structure at the mesoscale, namely via photoelastic force measurements and 3D $\mu$-CT study during compression and shear of granular materials and powders. The largest macroscopic scale of the flow is discussed in Section 2.3. A distinction is made between non-cohesive granular materials (analysed e.g. by particle image velocimetry - PIV or Positron Emission Particle Tracking - PEPT) and cohesive powders where the tracking of individual particles is extremely difficult due to small size. In this case, the flow properties properties are usually obtained via shear cells (bulk density and friction), FT4 device (powder flow energy), Freeman Lenterra Flow Sensor System for force measurements, rotating drum and the classical angle of repose test.

Besides experiments, the methods used to explore the micromechanical behaviour of particle systems involve numerical particle simulations and micro-macro transition methods, where the latter in general attempt to connect the particle scale with the process macroscale. In recent decades, the Discrete Element Method (DEM) that models the motion and interaction of individual particles has become very popular as a computational tool to model granular systems in both academia and industry. To date, not only due to increasing computer power available, considerable scientific advances have been made in the development of particle simulation methods, resulting in an increasing use of DEM. However, careful verification of the various numerical codes and validation of the simulation results with closely matching experimental data is essential to produce satisfactory quantitative predictions with added value for design and operation of industrial processes. One fundamental step towards this goal is the determination of the simulation parameters for the DEM particle model. This topic and the strategies to approach it are reviewed in Section 3.2.2, where the link with the microscale experiments is highlighted. Experiments need to be deployed (see Section 2.1), in order to measure particle-contact parameters and use them *directly* in particle simulations. However detailed contact information is only available for some materials such as glass spheres or rather large particles, whereas realistic, industrially relevant fine powders

can hardly be measured and contact level. In those cases, the microscale parameters must be inferred *indirectly* via comparison with simple lab scale element tests.
Once the numerical model has been calibrated and further validated, it can be used to study the mesoscale, and inform continuum models at the macroscale. In order to transfer information across the scales, some averaging or coarse graining techniques are required, that translate discrete particle data in continuum fields, as described in Section 3.4. Local macroscopic quantities such as density, velocity, stress and fabric can be extracted from the discrete simulation data (particle positions and velocities, interaction forces and torques). Note that both time- and space- averaging are required to obtain reasonable statistics, the latter being appropriate in the case of steady states. The methods and tools for this so called micro-macro transition are often applied to small representative volume elements (RVEs), where all particles can be assumed to behave similarly. Following the pioneer work by Goldhirsch, advanced numerical techniques have been developed in recent years, where the resulting coarse-grained fields exactly satisfy the momentum equations locally.
The final part of this section (Section 3.5) is dedicated to the representation of engineering setups directly via DEM simulations. These so-called mesoparticle simulations represent many particles as an entity, and as such catch the essential phenomenological features but are not directly related to the interaction parameters of the primary particles. A mesoparticle model is a valuable upscaling approach that allows for the simulation of large systems, including boundary values problems.

In spite of their versatile applicability and benefits, numerical methods have limitations such as excessive computational requirements, round off or truncation errors, and an intrinsic dynamic that sometimes does not reflect the experimental reality. Continuum models are still the most widely used to describe the process macroscale. Continuum mechanics theories solve the conservation equations for the whole medium i.e., the balance of mass, momentum and when necessary, energy. Although the balance laws are easily deducible, defining the constitutive relations poses the bigger challenge. Section 4 introduces the general rheological framework to describe the flow behaviour of granular materials and powders. The same section reviews existing granular rheological models derived using characterisation experiments as well as discrete simulations and micro-macro transition.
Classical approaches describe the flow rheology in terms of particle properties and system characteristics, like pressure or density, i.e., information attainable by conventional experiments in Sections 2.1 and 2.3. The kinetic theory in its standard form (SKT) is applicable in the very dilute regime, where the grains interact mainly through binary, instantaneous, uncorrelated collisions. Following the statistical mechanics approach, the generalization

of the kinetic theory of granular gases provides a meaningful hydrodynamic description, in accordance with the empirical Bagnold scaling between stresses and the square of strain rate. On the other hand, when the system is very dense, its response is governed by enduring contacts among grains, which are involved in force chains, that continuously rearrange during deformation. In these conditions, the granular material behaves like a solid, showing an elastic response in which stresses are rate independent. The corresponding flow regime is usually referred to as quasi-static. In the transition phase, where flows are dense, the grains interact via both force chains and collisions, and granular materials experience a phase-transition of - from a solid-like to a fluid-like Intensive studies on this topic have been conducted in the last decades. Recently, the French research group GDR-MiDi has suggested that dense granular materials obey a local, phenomenological rheology, known as $\mu(I)$-rheology, that can be expressed in terms of relations between three non-dimensional quantities: volume fraction, friction $\mu$, and inertial parameter $I$. This theory has been developed for ideal systems, made of rigid, perfectly elastic, monodisperse particles. Attempts for an extension of the $\mu(I)$-rheology to deal with soft, deformable particles, are also described. The rigorous STK and the phenomelogical $\mu(I)$-rheology are finally compared to empirical laws derived by laboratory and plant observations.

Section 4.3 is dedicated to the most recent theories, aimed to enrich the existing formulations with relevant features at the intermediate mesoscales, including permanent/transient fabric, structures and force chains.

In Section 4.3 local and non-local approaches to model granular heterogeneity are compared. The cooperative motion of grains causes the bulk properties at some location to be influenced by the flow taking place at all other locations. Works that belong to the first class assume that the flow can be described locally, when the appropriate set of state variables is identified, and their values in every material point are known. In the case of non-local approaches, a characteristic length scale is build directly into the model, as related the size of the grains themselves and the system properties, e.g. density. A number of other manifestations of finite-size effects in granular flows, with special focus on boundary effects, are finally highlighted.