Report of the IFPRI Powder Flow Working Group SAR30-08

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(in alphabetical order)

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1 Introduction

Michel Louge

The Powder Flow Working Group was charged by IFPRI to produce a review of research challenges on the flow of powders. It includes academics (Robert Behringer, Michel Louge, James McElwaine, Robert Pfeffer, Sankaran Sundaresan, and Jeorg Schwedes), industrial advisors (Karl Jacob, Thomas Halsey, James Michaels, and Paul Mort), and IFPRI officials (Nikolaas de Jaeger, Roger Place). The group held a meeting on October 21 and 22, 2004 in Newark, NJ to kick-off the activity. Triantafillos (Lakis) Mountziaris represented the NSF.

The group produced two principal deliverables. First, it wrote a series of short articles that are collected in this report. Second, for the NSF's benefit, it outlined broad research directions that the agency should consider to advance knowledge on powder flow that is relevant to industrial problems.

This report is organized from the small scale to the flow scale. Its articles summarize a state of understanding and recommend further work. We begin with considerations of interparticle forces; we then discuss the role of compressibility and cohesion in setting bulk properties; we focus on stresses; we explore similarity and scaling; we sketch numerical techniques; and we delineate regimes of granular flows. We close by discussing chute flows and by considering effects of the interstitial fluid.

2 Interparticle forces in powder flow systems

Robert Pfeffer

Interparticle forces, including van der Waals forces, capillary (liquid bridge) forces, electrostatic forces, forces leading to sintering and solid bridge formation, frictional forces, and

others, can have a strong effect on the behavior of powder flow systems such as hoppers, risers, packed and fluidized beds and pneumatic conveying. These forces are responsible for the cohesive properties of fine powders and their tendency to form aggregates or agglomerates. For these powders (primary particle size usually less than 30 μm), the interparticle forces are generally of the same order of magnitude or larger than the gravitational or hydrodynamic forces on the particles. Fig. 1 provides useful references on the subject.

2.1 van der Waals forces

The dominant interaction forces between particles in a dry powder are the electrostatic or van der Waals forces of attraction between molecules. Both Hamaker and Lifshitz quantified the van der Waals attraction forces for macroscopic bodies such as two spherical particles, and these are given by Eqs. 1 and 2, respectively

$$F_{vw} = \frac{AR}{12a^2} \tag{1}$$

$$F_{vw} = \frac{h\varpi}{8\pi a^2}\Big[1 + \frac{h\varpi}{8\pi^2 a^3 H}\Big], \tag{2}$$

where A is Hamakers constant, $h\varpi$ is the Lifshitz-van der Waals constant (values for most solids in air range from 1 to 10 eV), H is the hardness of the softer of the materials in contact, a is the surface separation which is of the order of the intermolecular spacing (0.165 to 0.4 nm) and R is the radius of the spherical particle. For materials with hardness above 10^5dynes/cm^2, the second term in Eq. 2 can be neglected and the two equations become identical with $A = 3h\varpi/4\pi$.

Using either Eq. 1 or 2, we find that the van der Waals force is of the same order of magnitude as the gravitational force for particles as large as 1 mm; yet these large particles are not cohesive, are free flowing and can be easily fluidized in a conventional fluidized bed. Thus it is apparent that the interparticle forces depend more on the particles surface properties than on the bulk, and a number of researchers have concluded that a measure of the particles surface asperities (usually taken as 0.1 μm) should be used instead of the particles radius R in Eqs. 1 or 2. This assumption causes the van der Waals forces to become independent of particle size, and reduces their magnitude so that they become of the same order as the gravitational forces for particles of about 80 μm, a much more reasonable size. Also, it is evident from Eqs. 1 or 2 that increasing the separation distance a between particles will decrease the van der Waals forces; this explains why the addition of fines or the adsorption of small molecules or the coating of nanoparticles onto the surface of cohesive powders will improve their flowability.

2.2 Capillary forces

Attractive capillary forces develop due to the formation of liquid bridges between contacting particles in the presence of vapors, e.g., water vapor, in the gas phase. Due to the close

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Figure 1: A sampling of papers on interparticle forces.

contact between particles in a powder, capillary condensation can occur at contact points even though the vapor partial pressure is less than the vapor pressure of the liquid. At a given temperature, the formation of a liquid bridge depends on the geometry of the gap between the contacting particles, the partial pressure of the vapor in the gas phase and on the properties of the solid-liquid system, i.e., contact angle, molar volume and surface tension and viscosity of the liquid. For porous particles, condensation in the pores will also occur.

For two spherical particles in the pendular state, the maximum static liquid bridge or capillary force is given by

$$F_c = 2\pi R\gamma \tag{3}$$

where γ is the surface tension of the liquid. Once again, the capillary force calculated for water using the particle radius R is much greater than the weight of the particle in the fine particle size range (<100 μm), and it is more realistic to use the size of the asperities. Even so, the maximum static liquid bridge force is appreciably larger than the van der Waals force. Also, liquid bridge forces, unlike van der Waals forces, can be adjusted by changing the amount of free liquid and its properties, and they are more complex than van der Waals forces because they can exhibit both static (surface tension) and dynamic (viscous) forces. Unlike the surface tension force, the viscous force always opposes relative movement and is quantified by a modified Stokes number, which can be used to predict whether surface-wet particles will coalesce in an agglomeration process, e.g., granulation in a fluidized bed.

2.3 Electrostatic forces

Electrostatic forces can also contribute substantially to the cohesion of particles and their aggregation by triboelectric charging (particle-particle contacts and particle-wall contacts) or by the formation of a potential difference when different types of particles are brought into contact. For triboelectric charging between a spherical particle of radius R having a charge Q interacting with an adjacent uncharged particle at separation H, the maximum electrostatic force on a particle is given by the classical Coulomb equation

$$F_{el} = \frac{Q^2}{16\pi\epsilon_0 H^2}\left[1 - \frac{H}{\sqrt{R^2 + H^2}}\right] \tag{4}$$

where ϵ_0 is the permittivity of vacuum. The electrostatic forces on a particle are usually less than the capillary forces for particles smaller than 100 μm and less than the van der Waals forces for particles smaller than 30 μm. Also, the Coulomb attraction forces are substantially reduced in a humid environment due to discharging of the system.

2.4 Sintering

The interparticle forces, which result in sintering or solid bridge formation, are quite different from those discussed above. Sintering is a time-dependent process where material

migrates due to a number of different mechanisms such as volume diffusion, surface diffusion, viscous flow or evaporation/condensation to the region of contact between two particles to form a neck. The size of the neck ξ, relative to the particle radius R, increases with time t, according to the equation

$$\left(\frac{\xi}{R}\right)^n = kt, \tag{5}$$

where n varies between 2 and 7 and k is a complicated parameter depending on the particular sintering mechanism. A sinter neck once formed can become permanent resisting any breakage forces caused by the movement of solids and gases in the powder flow system. The rate of material migration depends on temperature because migration is driven by surface energy minimization and is opposed by viscosity, which is highly temperature-dependent.

The result is that sintering occurs much faster at higher temperatures and the sintering temperature is usually much lower than the melting temperature of the particles. Thus the effect of temperature on sintering is quite different from its effect on dynamic liquid-bridge forces where high temperatures and reduced viscosity lead to lower forces, lower energy disruption in collisions and a lower rate of agglomeration. Sintering can lead to serious problems in powder flow systems, e.g., if a fluidized bed is operated at a temperature above the sintering temperature of the particles, the particles will bond together, form agglomerates, and the bed will quickly defluidize.

In addition to sintering, there is another class of processes during which solid bonds between small powder particles or granules form, usually during casual contact between particles. Here, the solid bond starts out as a liquid bridge, which subsequently solidifies, crystallizes or reacts chemically with the solid. The precursor of the solid bond may be a local melt which cools, a solution, which becomes more concentrated as the liquid evaporates or a slurry, which becomes more viscous as fine powder particles are absorbed into the bridge. Common examples are granulation of fine powders where small particles are held together by a binder and large permanent granules are formed during the process of drying, and caking of bulk powders during storage where a free flowing powder forms solid lumps due to moisture-induced agglomeration.

3 Bulk properties: compressibility and cohesion

Paul Mort

Compressibility and cohesion (or tensile strength) are bulk powder properties that greatly influence flow behavior. In this article, we consider:

[1] Characteristics of particles and their surfaces (i.e., micro-scale) and basic material properties that contribute to bulk compressibility and cohesion;

[2] A general paradigm linking compressibility and cohesion with the machine-scale environment and the resulting powder flow behavior;

[3] Correlations between compressibility and cohesion for various classes of powder and granular materials.

3.1 Particle Characteristics and Material Properties

A list of basic particle characteristics and material properties that influence the powder compressibility and cohesion is shown for granular, moist granular and fine powder classes in Fig. 2. The relative importance of each property or characteristic depends on the type of powder and/or product application. Detailed characterization of particles (size, shape, roughness, etc) and their material properties (complex modulus, yield strength, dielectric permittivity, etc.) can be considered as the fundamental microscopic base for understanding bulk powder behavior. While there has been considerable progress toward the linkage of particle-scale characteristics with bulk powder behavior, it is clear that much work needs to be done to better elucidate the functional relationships between particles and the bulk, especially for particles with distributed characteristics.

Further, the effects of particle size, size distribution and pre-consolidation on bulk flow are not apparent from single-particle characterization; rather these bulk effects depend on ensemble particle packing and may require an intermediate scale of scrutiny (i.e., a meso-scale) combined with statistical mechanics to enable useful linkages between micro-scale characteristics and bulk flow behavior. For a more detailed discussion of the linkage between micro-scale particle properties and bulk powder flow, the reader is referred to the recent work of Jones et al. [1], [2], which offers parallels between micro-scale analyses of inter-particle friction and bulk flow yield loci.

3.2 Powder Flow Paradigm

Consider a simple paradigm for flow in terms of a driving force relative to a flow constraint as shown in Fig. 3. In an industrial application, the driving force is provided by the unit operation such as gravity flow in a hopper, pressure in a pneumatic conveying line, a mechanical agitator in a mixer, etc. The driving force creates a shear stress in the powder τ and results in a powder flow that is characterized by a shear rate $\dot{\gamma}$ and other detailed flow characteristics that depend on the flow regime and scale of scrutiny used to measure the flow (Fig. 4).

Flow constraints include both extrinsic and intrinsic components. Extrinsic constraints are defined by physical volume constraints (e.g., converging walls in a hopper) as well as stress constraints (e.g., a consolidation normal stress due to an overburden). Intrinsic constraints are associated with the powder itself, chiefly the compressibility and cohesive bulk properties along with the more fundamental particle characteristics and material properties. The relationship between the driving force and the flow constraints are described

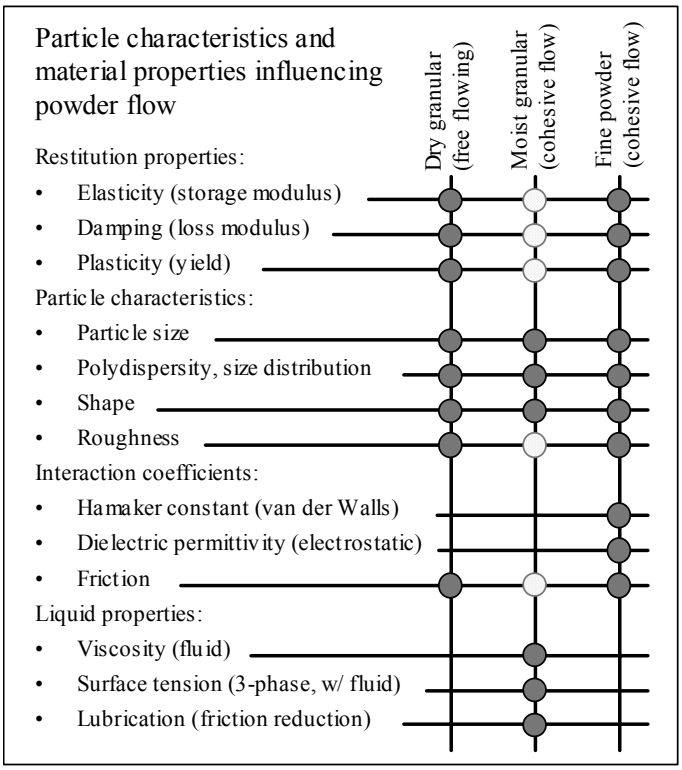

Figure 2: Overview of particle characteristics and material properties affecting the various types of bulk flow behavior. The darker connection points indicate significant relationships. In the case of the moist granular materials, the significance of the lighter shaded connections for solid restitution and frictional interactions may be eclipsed by the viscous dissipation and lubrication effects of the added liquid.

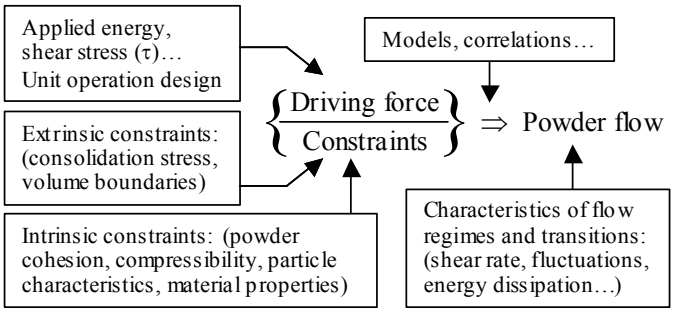

Figure 3: A general paradigm for powder flow as a function of a driving force relative to flow constraints.

in models and correlations that are used to predict flow behavior. Models based on bulk properties including compressibility, cohesion and bulk yield strength are more routinely used as quasi-predictive tools for flow behavior, and are regularly employed in the design and scale-up of industrial unit operations for powder processing as well as overall powder handling systems. Continuum models for both incompressible and compressible powders are reviewed by Tardos and Mort [4].

3.3 Correlations between Compressibility and Cohesion

A conceptual correlation between powder compressibility and tensile strength is illustrated in Fig. 5. A similar diagram has been proposed to compare packing density and frictional angle of repose [5].

On the top half of the diagram, the relatively incompressible materials are typically granular in nature, relatively coarse in particle size (i.e., > 100 μm) and assembled in a relatively dense state of packing (e.g., >60 vol% solids). The bottom half of the diagram represents compressible materials; these materials characteristically increase in bulk yield strength as they are compressed. On the right side of the diagram are materials with intrinsic tensile strength that provide resistance to shear even if there is no normal force acting to compress the powder.

Materials in Fig. 5a, such as dry sand and glass beads, are often been used as model materials in scientific studies. Numerous studies have used glass beads as a way to test interactions with minimal inter-particle forces (friction and tensile forces), and to compare these results to models of frictionless hard spheres. Comparing sand to glass beads offers a way to explore the effects of changing bulk friction without significantly affecting tensile interactions between the particles.

In Fig. 5b, cohesion can be induced by mixing or adsorbing a small amount of liquid onto the surface of a granular material. The presence of liquid bridges between particles

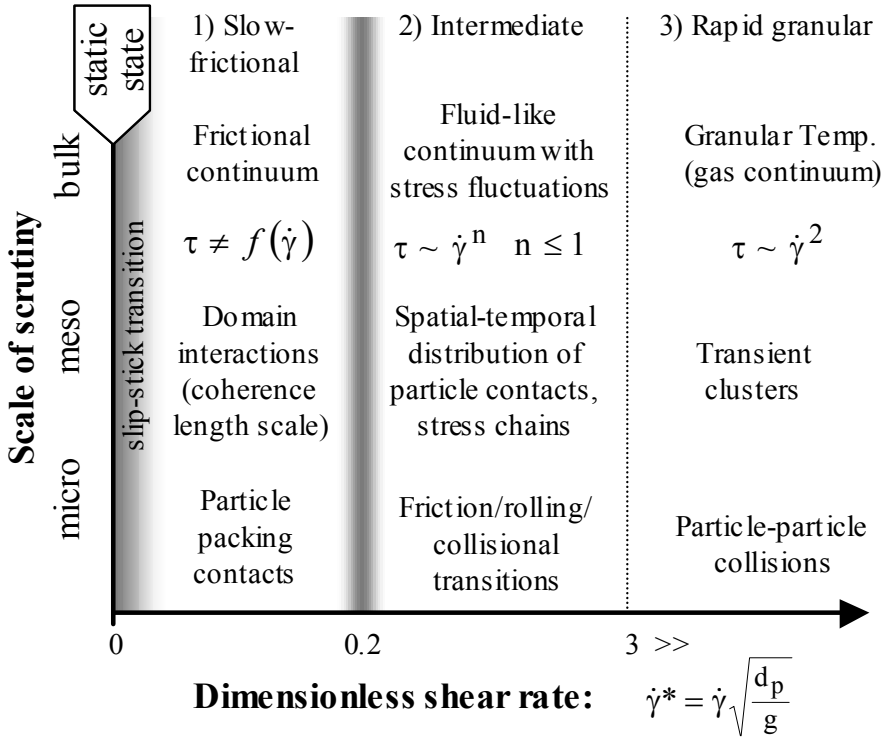

Figure 4: Flow regime diagram (IFPRI Powder Flow Workshop, Bremen, 2003; based on [3]) showing the static state, three flow regimes (slow-frictional, intermediate and rapid granular) and tentative boundaries between the regimes. The regimes are distinguished using a dimensionless shear rate. Physical features of each regime noted across a scale of scrutiny including particle and particle surface interactions (micro), particle clusters and chain assemblages (meso) and bulk flow behavior (macro). In section 5.1, we provide a more physical way to make the shear rate $\dot{\gamma}$ dimensionless using the parameter $I = \dot{\gamma}d/\sqrt{P/\rho_0}$.

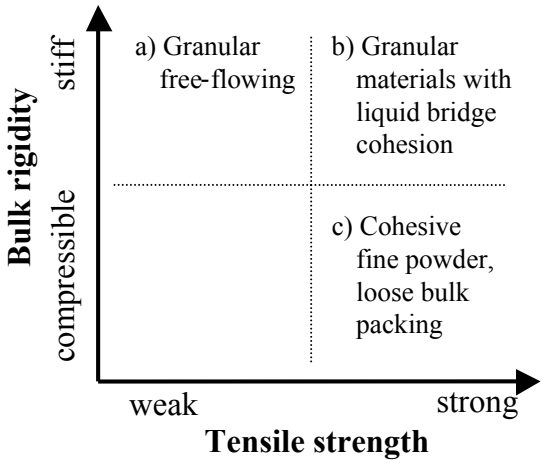

Figure 5: Correlations in bulk powder properties relevant to flow, showing general relationships between bulk compressibility and inter-particle forces (tensile strength or cohesion). Powder compressibility is key to flow behavior, especially in volume-constrained flows, i.e., where dilatent powders may give rise to high stresses in the flow. Sources of cohesion include inter-particle forces in fine powders (e.g., van der Waals, electrostatic forces) and liquid bridging in moist granular materials.

provides tensile strength and the effect of cohesion. This is a popular way to study cohesive interactions, since the amount of added liquid can be controlled experimentally. In addition, this approach is more amenable to simulation since the granular particles are relatively coarse mass elements, making it possible to simulate the system using a reasonable number of discrete particles. On the other hand, the presence of liquid adds complexity to the analysis of a developed flow, including viscous interactions and lubrication. In general, moist granular materials can be arranged into relatively dense packing arrangements leaving little free volume for compression. Such materials are often dilatent and will volume-expand under applied stress (e.g., wet sand on a beach).

In Fig. 5c, a great many industrial powders pose a challenge for powder flow. Bulk-compressible materials are more often in a loosely packed state, for example, where packing is inhibited by cohesive interactions in a fine powder. These cohesive interactions are caused by inter-particle forces (van der Waals, electrostatic, other contact bridging effects of humidity, hydration, etc., see section 2), which are significant compared to gravity acting on the fine particles. Under typical packing arrangements, the bulk density of a cohesive fine powder is low compared to its solids density, and the excess inter-particle porosity provides room for consolidation under applied pressure. It is generally accepted that fine cohesive powders act as loose clusters across a coherence length scale. This adds an additional level of spatial interaction, i.e., a meso-scale.

While there are many empirical studies of fine powders in the literature, the linkage of experimental work on fine powder with simulations are much less common. Simulations of fine cohesive powders are also more challenging because of the large number of fine particles required to capture the interactions across the coherence length scale. In addition, there are considerable experimental challenges in the controlled manipulation of the inter-particle forces. As an additional complication, fine powders with added moisture (not shown) have two mechanisms of cohesion, and can exhibit time-dependent flow properties that are difficult to predict.

4 Stress and Flow Fields in Particulate Flows

Robert Behringer and Paul Mort

Industrial practitioners rely on routine handling of powders and granules for many bulk solids processes such as accurate feeding into a pressing operation, precise packaging, bin storage, reliable conveying and other handling operations. Productivity and plant reliability are often limited by solids handling [6].

In addition, practitioners are regularly asked to develop and scale-up processes for making powdered or granular products with critical quality attributes that are rooted in a micro-scale of scrutiny. Examples include micro-scale compositional variance in a multi-component mixture, the microstructure of granules made by an agglomeration process, the mesoscale structural fabric of in a perform for a particulate-filled composite, or the effect of die filling on the structure of a pressed piece or tablet.

In the context of industrial handling and processing, we consider dry particulate flows to include:

[1] granular materials that are relatively incompressible and non-cohesive;

[2] granules that may and exhibit cohesive behavior, e.g., by adsorbed moisture or other liquid capable of forming liquid bridge adhesion between particles;

[3] finely powdered materials that are both compressible and cohesive (e.g., due to van der Walls interactions) and may also include interactions due to adsorbed moisture.

In this brief, we seek to elucidate the linkages between the fundamental physics of stress and flow fields in dry particulate flows and industrial needs outlined above. This includes multiple scales of interaction in the flow, i.e., among individual particles, clusters thereof, and between the bulk flow and the system constraints or boundaries imposed by the process unit operation. Further, we consider the effects of stress fluctuations across this range of interaction scales as well as the integral effect of stress and flow fields on cumulative energy dissipation in processes with particulate flows. We also consider the issue of history dependence and variability.

A variety of shear configuration have been discussed in the physics and engineering literature, including plane shear, annular shear, chute flow (vertical and inclined plane), hopper flow, heap flow and cascading flow in a rotating drum. There are many references spanning the combined literatures that consider aspects of granular flows in these various configurations, or that consider fluctuations, force transmission and related phenomena; a brief sampling of papers on the subject is shown in Fig. 6 and 7. Recent IFPRI projects have investigated aspects of the Couette flow and agitated U-tube geometries [7], [8], and there was much discussion in the IFPRI Powder Flow Workshop (Bremen, 2003) concerning appropriate test geometries [9].

In the current discussion, we consider the industrial scale-up problem in a mixer or mixer-granulator as illustrative of the importance of a multi-scale approach. In many cases, the starting point in an industrial process development is a small amount of material (maybe a few grams or kilograms) and the production scale will be many times larger (in mixers that can be hundreds or thousands of liters in volume). Current industrial capability in a mixer operation is to measure global process indicators like power draw (`kW`) and specific energy (`kJ/kg`); however, we don't easily differentiate these into distributed constituents of flow and stress fields. While one may endeavor to maintain similar power ratios and/or specific energy inputs across bulk scales, the distributed local stress and flow fields and fluctuations (in space, in time, and with repetition) thereof may not necessarily scale in a similar way; e.g., a bigger mixer may have a broader distribution of these fields (more work in some regions, less in others) compared to the lab or pilot scale. If the product attributes are too sensitive to these local differences, the scale-up may fail.

How do we reconcile the measurable process indicators like power consumption to the stress and flow fields in a mixer? Are there other useful indicators besides those in current use, such as instantaneous power that would provide useful diagnostic information?

As a way forward that is both industrially and scientifically relevant, a combined approach including experimental investigation, simulation and development of theory may be fruitful. Several possible cases studies are suggested:

[1] Generalized Couette flow is amenable to detailed experiments under highly controlled steady-state conditions. As such, this type of flow can provide detailed information on flow properties, scaling etc.

[2] Centripetal flow with a controlled shear field and tunable material properties can be viewed as an extension of Couette flow to a mixing application at higher shear rates. While there have been a number of recent computational and experimental studies on flow patterns in mixers and mixer-granulators [10], [11], [12], [13], it is reasonable to focus initially on a relatively simple geometry with a vertical axis of rotation and a friction plate to impart a relatively uniform shear field to the particles [14]. The broad band of fluid-like shear in this geometry is similar in some respects to the recent granular flow fields generated in a modified Couette-like geometry by

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Figure 6: A sampling of papers on powder flows.

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Figure 7: A sampling of papers on powder flows.

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[3] A third possible case study is flow through an orifice, as in but not limited to hopper flow. Again, this system offers the possibility of detailed experimental probes, and at the same time it is highly relevant to a broad range of industrial applications. Notably, these are suggested case studies. Other systems of configurations would also be relevant both to industrial applications and to probes of science. The choice of a case study should offer industrial relevance, the possibility of high quality experimental and computational probes, and very importantly, the possibility to explore the role of scale.

A key issue that is common to the above case-study approaches is size-scaling. This is also addressed in section 5 from the standpoint of dimensional analysis. In order to tease apart this problem, it is important to address the following:

[1] What sets the stress and flow fields for the relevant flow regimes? How are stress changes or changes in other quantities transmitted throughout the sample?

[2] How are these related to boundary conditions, particle properties, and control parameters?

[3] How should one characterize a granular mixture, particularly one where the particles have a continuous range of sizes, shapes and/or surface properties? Given that real granular materials may require a very large number of parameters for a complete physical description, what are the most useful truncations of such a parameter space that give reasonably accurate characterization?

[4] What is the range of states that is compatible with a given set of (boundary) control parameters? The answer to these will address the repeatability issue.

[5] What is the character of fluctuations that occur in stresses/forces and flow fields? What mathematical approach can be used to incorporate these fluctuations into a suitable theory (e.g. Langevin approach for random uncorrelated fluctuations, extended granular temperature similar to Eq. 12, etc.).

[6] Is there a connection between the possible states consistent with a set of control/boundary conditions, and the range of fluctuations seen? That is, is the nature of repeatability tied to fluctuations?

[7] What is the response of a system to a change at the boundaries?

[8] In a dynamical process, what is the relation between energy input and flow?

[9] What parameters control the transition(s) between different granular states, e.g. quasi-static vs. intermediate? What is the nature of these transitions?

[10] What experimental models would be most useful in a) addressing basic physical questions, and b) providing key insights for practical applications?

[11] What diagnostics can be used to infer information of flow fields and stresses both internally and at the boundaries?

Specific case studies should address some set of the above questions. They should be industrially relevant, and accessible to experiment and simulation. Ideal studies would include both these last two components. Studies should point in the direction of developing new modeling approaches. They should also consider the effects of varying size scales. This last point is of importance for several reasons. First, scale variations can provide important insights into the nature of the physics involved. And scale-up remains one of the most challenging problems for industrial applications.

5 Scaling in Cohesive Flows

James McElwaine and Paul Mort

Perhaps the biggest difficulty in powder technology is scaling. How does one upscale a process that is tested and developed with a few kilogrammes of material to one that uses tons? Scaling issues in physics are addressed by Buckingham's Pi theorem, which states that physical laws are independent of the choice of units. Thus the correct scaling can be obtained by keeping all the non-dimensional groups that can be formed from the relevant dimensional quantities constant. This approach is extremely successful in classical fluid dynamics, where similarity, based on Reynolds number for example, generally provides very accurate scaling between laboratory experiments and full-scale flows.

d	[L]	particle diameter
m	[M]	particle mass
g	[LT^{-2}]	gravity
L	[L]	experiment size
U	[LT^{-1}]	experiment velocity scale
ω	[T^{-1}]	experiment angular velocity
ρ_0	[ML^{-3}]	$\propto m/d^3$, bulk density

Table 1: External Parameters.

The great difficulty with granular matter is that it is normally impossible to keep all the non-dimensional groups constant. Often this is because we do not want to change

the particle properties, such as size, when we scale. Scaling of granular flows in particle processing operations can then be considered in several ways: 1) on a bulk scale, to ensure that the same flow regime or combination of flow regimes exist; 2) on a particle scale, to ensure that the relevant non-dimensional groups are similar within each flow regime; and 3) that the exchange of particles between flow regimes also follows similarity of temporal and spatial residence distributions. In this section, we discuss scaling for fixed particles in situations of practical importance, such as mixers. While we consider three main flow regimes (slow-frictional; intermediate and rapid granular flows), the focus is on industrially-relevant dense flows in the frictional and intermediate regimes. Further, in consideration of cohesive materials where interparticle forces dominate over fluid-particle drag forces, we ignore the interaction with the ambient fluid.

5.1 Dimensional Quantities

$\mathbf{u}$	$[\mathrm{LT}^{-1}]$	velocity
ρ	$[\mathrm{ML}^{-3}]$	density
σ	$[\mathrm{ML}^{-1}\mathrm{T}^{-2}]$	stress tensor
$\dot{\gamma} = \frac{\partial u_x}{\partial y}$	$[\mathrm{T}^{-1}]$	shear rate

Table 2: Flow variables

Table 1 contains the basic parameters that can be used to to describe a flow situation. From these other quantities such as shear rate, $\dot{\gamma}_0 = U/L$, can be defined. We want to consider scalings where the particles are not changed so that m and d are constant. The only flows that can remain self similar then as L changes will be those independent of the non-dimensional group $N = L/d$, the size of the experiment in particles.

Energy is typically imparted to granular flows through the boundaries and is dissipated by various damping mechanisms (frictional, viscous, plastic deformation) associated with particle collisions. The simplest theory for energy dissipation applies to dilute, high energy flows where kinetic theory can be used to describe the granular system. In this regime, the fluctuation energy is the analogue of temperature. (It is called "granular temperature" and is defined in Eq. 12 of section 8). However, this theory is not generally applicable to industrially-relevant systems because of inelastic collapse and the effects of gravity. Except for thin flows where $N = L/d \approx 10$, fluctuation energy will decay exponentially away from the boundaries with a length scale $\propto d$. Thus to maintain an inertially dominated regime, where kinetic theory is valid, the input energy needs to increase exponentially with N. This only permits scaling over a very narrow range as at higher energy the particles will be destroyed. This argument is valid for the case where fluctuation energy is mostly created at the boundaries, but does not hold for the shear production of fluctuation energy, which can occur throughout the bulk.

A more general scaling approach is needed to describe flows in dense regimes and at

lower internal energies. The non-dimensional group $I = \frac{\dot{\gamma}_0 d}{\sqrt{P/\rho_0}}$ (P is the pressure) can be thought of as the ratio of microscopic inertial forces to confining forces, if the velocity fluctuations are proportional to the shear rate. It was first introduced by the GRD Midi [16] to reconcile data from a wide variety of granular flows (shear cells, chutes, rotating drums, etc.). Thus large I corresponds to the kinetic regime and small I to a regime dominated by continuous contacts. Intermediate values of I correspond to dense flows where both friction and collisional interactions are relevant. Many industrially-relevant flows occur in this intermediate region. It is a more physical parameter than $\dot{\gamma}\sqrt{d/g}$ shown as the abscissa of Fig. 4.

In free surface flows an important non-dimensional group is the Froude number $\mathrm{Fr} = U/\sqrt{gL}$. This can be thought of as the ratio of the mean flow velocity to the speed of surface waves. When $\mathrm{Fr} < 1$, *subcritical* flows, the flow downstream can effect the flow upstream, but when $\mathrm{Fr} > 1$, *supercritical* flows, downstream conditions cannot effect the flow upstream. For a flow to scale correctly therefore Fr must be kept constant, or very low, or very high.

Rotating systems frequently occur industrially such as mixers. If a drum has radius L and rotates with angular velocity ω then the centripetal acceleration is $L\omega^2$ and we can define the acceleration ratio $A = L\omega^2/g$. When A is large gravity becomes unimportant and the body force experienced by the flow is dominated by centripetal acceleration. In this case there are different approaches to defining the Froude number. If one takes $U = L\omega$ then $\mathrm{Fr} = \omega\sqrt{L/g}$ (sometimes the definition $\mathrm{Fr} = \omega^2 L/g$ is also used), but Fr is no longer the ratio of flow speed to wave speed. If one wants to keep this interpretation then the local acceleration is set by $L\omega^2$, so that $\mathrm{Fr} = \omega L/\sqrt{(L\omega^2)L} = 1$ and these flows will always be on the supercritical/subcritical transition point and scale automatically.

When $A \gg 1$, I is also effected by rotation since the pressure will be given by $P = (L\omega^2)L\rho_0 = L^2\omega^2\rho_0$, thus $I = \dot{\gamma}d/(\omega L)$. In this case, the predicted scaling of I depends on the length scale used in the calculation of $\dot{\gamma}$. If we adopt particle length scales in the numerator (i.e., velocity fluctuations scale with $U/d = \omega L/d$) then we predict $I = 1$ regardless of scale. If however the shear is distributed over the length scale L then $\dot{\gamma} = U/L = \omega$ so that $I = 1/N$. Thus as the size of the system increases we move towards a frictional regime. To further probe the nature of inertial behaviour, we may need additional scaling groups to describe micro-scale interactions among particles and clusters thereof. Contact time ratios, coordination numbers, Stokes Numbers and stiffness ratios have been suggested in the literature.

5.2 Dynamical Similarity

In the previous section we have seen that microscopic inertial effects must be small so that kinetic theory type rheologies are inappropriate. That does not mean however that macroscopic inertial effects are unimportant. Momentum conservation, without body forces, can

σ_s	$[\mathrm{ML}^{-1}\mathrm{T}^{-2}]$	shear cohesive stress
σ_t	$[\mathrm{ML}^{-1}\mathrm{T}^{-2}]$	tensile cohesive stress
ν	$[\mathrm{ML}^{-1}\mathrm{T}^{-1}]$	dynamic viscosity
μ	$[\cdot]$	Coulomb friction

Table 3: Possible Constitutive Parameters

be written

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla(\rho \mathbf{u}\mathbf{u}) = \nabla \sigma, \tag{6}$$

where the variables are defined in Table 2. When microscopic inertial effects are small density fluctuations are also small so we let $\rho = \rho_0$. We use the quantities from Table 1 to scale equation 6 (e.g. $t = L/U\tilde{t}$)

$$\frac{\partial \tilde{\mathbf{u}}}{\partial \tilde{t}} + \tilde{\nabla}(\tilde{\mathbf{u}}\tilde{\mathbf{u}}) = \frac{\sigma_0}{\rho_0 U^2}\tilde{\nabla}\tilde{\sigma} = \frac{1}{\mathrm{Re}}\tilde{\nabla}\tilde{\sigma}, \tag{7}$$

where $\tilde{\cdot}$ is used to denote a non-dimensional variable, and σ_0 is a representative stress. Re is a generalised Reynolds number. If Re is very large or very small then it need not be constant for similarity, since either inertial or dissipative stresses dominate respectively. For intermediate cases however it must be kept constant for similarity.

To progress further it is necessary to have a constitutive relation that determines the stress in terms of other flow variables. For simplicity we assume locally a simple shear flow $\mathbf{u} = (\dot{\gamma} y, 0, 0)$ and concentrate on the shear stress term σ_{xy} and normal stress σ_{yy}. A reasonably general rheology that includes, frictional, cohesive and viscous stresses can be written

$$\sigma_{xy} = \mu \sigma_{yy} + \sigma_s + \nu \dot{\gamma}, \tag{8}$$

where the new variables are defined in Table 3. When $\mu = 0$ this corresponds to a Bingham rheology. If $\nu = 0$ we have a cohesive Coulomb rheology. If $\mu = 0$ and $\sigma_s = 0$ we have a Newtonian rheology. In general however all three terms will be important in different parts of the flow and ν will be a function of the flow variables (proportional to a power of $\dot{\gamma}$ for Herschel-Bulkley rheology for example). Re can be regarded as the harmonic sum of three contributions from frictional, cohesive and viscous force $1/\mathrm{Re} = 1/\mathrm{Re_f} + 1/\mathrm{Re_c} + 1/\mathrm{Re_v}$ Near moving boundaries the local shear will be high and viscous effects will dominate so $\mathrm{Re} \approx \mathrm{Re_v} = \frac{\rho_0 U^2}{\nu(U/L)} = \frac{\rho_0 U L}{\nu}$. In freely falling parts of the flow cohesive stresses σ_s and σ_t will hold the particles in lumps and $\mathrm{Re} \approx \mathrm{Re_c} = \frac{\rho_0 U^2}{\sigma_s}$. In other regions of the flow the confining pressure, $P = \sigma_{yy}$, may be large and cause friction to be the main component of stress so that $\mathrm{Re} \approx \frac{\rho_0 U^2}{\mu \sigma_{yy}} = \frac{\rho_0 U^2}{\mu g' \rho_0 L} = \frac{\mathrm{Fr}^2}{\mu}$. There is also a connection with I since in the kinetic regime $\nu \propto \dot{\gamma} \rho_0 d^2$ so that $I^2 \propto \mathrm{Re_f}/(\mu \mathrm{Re_v})$. Reynolds number similarity is often achieved in fluid dynamics experiments by changing the fluid viscosity as U and L

vary. But for fixed particles this cannot be done and similarity will only occur if ν has a fortuitous dependence on U and L.

Of great practical concern are quantities such as the energy dissipated in a system. This is the integral of stress times strain over the volume of the system, which scales as $\sigma_0 \dot{\gamma} L^3 = \rho_0 U^3 L^2/\mathrm{Re} = \rho_0 g^{3/2} L^{7/2} \mathrm{Fr}^3/\mathrm{Re}$. The difficulty is that it is not possible to keep Re constant in a flow.

$N = \frac{L}{d}$	size in particles
$I = \frac{\dot{\gamma} d}{\sqrt{P/\rho}}$	non-dimensional shear
$\mathrm{Fr} = \frac{U}{\sqrt{gL}}$	Froude number
$\mathrm{Re} = \frac{\rho_0 U^2}{\sigma_0}$	Reynolds number
$A = \frac{L\omega^2}{g}$	Acceleration ratio

Table 4: Non-Dimensional Groups

5.3 Scaling challenges

The multiplicity of length scales in granular and powder flows complicates the use of classical scaling approaches such as the Buckingham's Pi Theory. Specifically, it is difficult to scale the macro-system while maintaining constant attributes on the particle scale. In addition, there are other length scales that further complicate the situation including particle cluster scales (both spatial and temporal), fluctuation decays and scales associated with transition layers and discrete flow regimes within an overall system. While it may be possible to maintain similarity of certain groups such as Froude Number and, in some cases shear rate, it is not possible to maintain the particle number and its associated non-dimensional groups. A generalised Reynolds number is proposed as a descriptor of the flow rheology; it can be used to describe various dissipation mechanisms including friction, viscous damping and cohesive interactions, each of which may be dominant in different regions of the flow. While it is generally not possible to maintain Fr, I and Re on scaling, one may use the tactic of maintaining one or more of these at very high or very low numbers in order to create a more homogeneous flow regime. More generally, a detailed analysis of the flow is necessary to divide it into regions and boundary layers where the different forces dominate. The great challenge is to do this for complicated flows and then apply the appropriate scalings to each region.

6 Numerical tools

James McElwaine

Particle flows can be considered on many different scales, each appropriate for a different purpose. At the smallest scale the molecular properties and surface structure of the particles can be considered. However, the size of the systems to be modelled for practical problems dictates that a continuum model is used. The question is then how to go from the small scale knowledge of the physics to a model that can be run in reasonable computer time in realistic scenarios. This problem is far from solved for granular systems, but in this section we sketch some of the relevant techniques.

6.1 Discrete Element Method

The DEM (Discrete Element Method) is a direct approach for modelling particulate systems, whereby each particle is treated individually. It is well developed and conceptually very similar to molecular dynamics. In special cases, when there are no continuous contacts, a particularly fast algorithm can be used that treats collisions as instantaneous, but this is rarely applicable even for non-cohesive flows. The other approach involves a contact model that determines the forces between two particles in contact. This model can be very general and include cohesion as well as history dependent terms. These methods require computational time proportional to the number of particles divided by the collision time. For spherical particles a million can be simulated on an ordinary workstation. However, for non-spherical particles many fewer can be simulated, and realistic systems contain 10^9 particles. Thus direct simulation at the particle level is in the range of current supercomputers for spherical particles, but this is not cost effective and is likely to remain impossible for the next decade for larger systems or those containing non-spherical particles. These simulations are primarily useful for developing and validating continuum models.

6.2 Continuum Models

If we assume that the properties of a flow are not varying too rapidly over lengths of the particle size we can hope to use a continuum model that averages over these scales. Conservation of mass and momentum then lead to the Eqs.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\mathbf{u}\rho) = 0 \tag{9}$$

$$\frac{(\partial \mathbf{u}\rho)}{\partial t} + \nabla \cdot (\mathbf{u}\mathbf{u}\rho) = \mathbf{g}\rho + \nabla\sigma, \tag{10}$$

where ρ is the density, $\mathbf{u}$ the velocity, $\mathbf{g}$ gravity, and σ the stress tensor. This needs to be supplemented by a constitutive relation and equation of state that determines σ in terms of $\mathbf{u}$, ρ and possibly other variables such as as granular temperature (defined in section 8). The numerical solution of equations of this form has been well studied in Computational Fluid Dynamics and the methods used can be divided into three broad types. In the structured grid method the equations are discretised on a fixed set of points such as a Cartesian grid. This results in simple and efficient codes, but is less good for complicated geometries

and free surfaces. The Finite Element Method uses an unstructured grid that exactly fits boundaries and can evolve with them. It is more complicated to use especially with free surfaces. There are also grid free approaches such as Smooth Particle Hydrodynamics. This is similar to DEM in that blobs of the material are modelled and allowed to move, but their equations of motion are derived from Eqs. 9 and 10 . The method is of low accuracy, but straightforwardly applied to free surfaces and can include cohesion. In particular it can easily cope with topology changes that might occur as a mixer blade moves through material.

6.3 Perspectives

There is no one modelling approach that allows the direct simulation of industrial particulate systems. However a hierarchy of simulation techniques can be used to bridge the different scales. Knowledge of the inter-particle contacts can be used to run DEM simulations in simple geometries with reasonable numbers of particles. These simulations can be used to develop and validate boundary conditions, constitutive relations and equations of state for continuum models. These can then be simulated for full sized industrial systems.

7 Different Regimes in Granular Flows

James McElwaine

Granular materials are sometimes called a fifth state of matter as they can behave like solids, liquids and gases depending on the situation. Many important industrial flows can contain all these states in different regions. For example a discharging hopper may contain entirely static regions, flowing regions and empty regions. To accurately model and predict such flows progress is needed in three areas: the physics of the bulk and interface regions must be characterised by careful experiments, the mathematical nature of the equations must be understood so that appropriate boundary conditions can be chosen to give well-posed problems, numerical techniques must be developed for dealing with multiple phases.

7.1 Continuum Theories

If the constitutive relation, equation of state and boundary conditions are known for a system then in theory this system can be solved directly without dividing the system into different regions. In practice such an approach is computationally prohibitive and frequently ill-posed. Instead the system must be dynamically split up into regions where different states exist and a solver used in each region with the appropriate boundary conditions between them. Provided that the boundary regions are sufficiently thin we can expect good results. The questions then to be answered are the following: What determines the location and movement of these boundaries? How are mass and momentum transported

across them? For a Newtonian liquid-gas mixture below its triple point separating a system into two parts with a boundary between them is natural because the thickness is on the molecular lengths scale. If the liquid phase boils this will become extremely difficult as bubbles appear and the topology of the surface separating the two phases becomes complicated. A direct solution where the same equations were solved throughout the mixture would be extremely hard to implement however as the equations would be extremely stiff on the boundary. Above the triple point there is no distinction between liquid and gas, the boundary region is the entire system, and a direct solution would be appropriate. Analogous situations occur in granular flows and here the boundary between solid-like and fluid-like phases may also be poorly defined.

7.2 Solid-Fluid Boundary

A simple flow with solid-like and fluid like behaviour is a heap of granular material. If material is slowly added to the top, from time to time avalanches of varying size will occur, carrying the material down and maintaining the slope angle close to the angle of repose. If we consider the positions of all the grains before and after an avalanche, then we can define the flowing part, at any time, as consisting of all grains that are not in their initial or final position, though other definitions maybe more useful in come cases. Erosion (entrainment) and deposition processes lead to the transfer of particles across the boundary and its movement. There are a wide range of physical mechanisms that can cause erosion including impacts, abrasion, ploughing and blasting. These processes are all poorly understood and experiments would be of great value. Assuming that the interface between the regions moves smoothly, which is not necessarily the case especially when cohesion can cause regions to move in a solid like fashion, the interface can be tracked forward in time using a variety of methods such as marker-in-cell or level-set. Mechanisms such as abrasion probably require additional variables to track the bond strength between particles in the solid-like phase.

Typically in a continuous flow on a heap there is a thin surface flow with continuous motion and a much deeper stochastic flow where the particles are mostly stationary but make small jumps. These thus have an average velocity which in some experiments decays exponentially with depth. If we wish to make a model that can include this behaviour there are two approaches. The approach outlined above will fail as there is no clear boundary. There are several solutions. One can simply ignore these small particle motions. One can go back to solving for the complete system where the flowing and stationary regions are not separated. One can include the stochastically moving particles in a solid phase model where they are allowed to move like dislocations. Or one can construct a model that is unstable or stochastic so that the lower boundary moves backwards and forwards even for *steady* boundary conditions. This then allows the recovery of smoothly decaying mean velocity. This approach is probably best fundamentally as it is physically realistic and may also be able to generate the initial avalanche flows. However, for practical purposes it is

probably best to include these particles in the solid region, by defining the moving region as only those particles that are moving for a certain fraction of the time, and then to ignore motion in the solid phase.

7.3 Perspectives

The difficulties in simulating flows with different phases and sharp boundaries are considerable, particularly when there is intermittent motion. There are methods available that can overcome these difficulties, but the greatest problem is lack of data to verify them. Careful experiments on cohesive erosion and deposition processes are urgently needed.

8 Flows down inclines

Michel Louge

In this section, we illustrate questions raised in previous articles by providing examples of powder flows involving particles and geometries simple enough for theory to predict flow behavior. We focus on dry, dense granular "chute" flows of spheres on rough and flat inclines, for which the granular community is currently achieving rapid progress.

Dense dry flows of spherical grains down inclines depend crucially on the nature of the base, the presence of side walls, and the thickness h of the flow. Here, we summarize salient observations made in laboratory experiments and numerical simulations on flat and rough bases. We also refer to theories that have captured these observations.

Each kind of flow possesses a different range of angle of inclination $\alpha \in]\alpha_{min}, \alpha_{max}]$ in which velocity and thickness are steady and fully-developed (SFD) on time and length scales much longer than the inverse shear rate and the flow thickness. In the absence of side walls, SFD momentum balances in the directions x along the flow and y perpendicular to the base set the effective friction of the flow μ_{eff} at any depth as the ratio of the shear stress S and normal stress N on surfaces at constant y,

$$\mu_{eff} \equiv \frac{S}{N} = \tan\alpha. \tag{11}$$

The challenge to theory is to predict the resulting mass flow rate in terms of h and parameters characterizing the grains and the boundaries.

Measurements are limited in three-dimensional dense granular flows. Once the inclination is set to better than $\sim 0.1^\circ$, the overall mass flow rate is typically found by weighing the output collected over a known time, and the height is recorded with a laser [17]. Unlike powder flows involving electrostatics, cohesion, or other forces mentioned in section 2, the scaling is relatively straightforward. The mass flow rate is made dimensionless with $\rho_s\sqrt{gd}Wd$, where ρ_s is the material density of the grains, d is their diameter, g is the

acceleration of gravity and W is the distance between the lateral walls that bound the channel.

Other techniques include capacitance probes, which record instantaneously the dimensionless "mass holdup" $H^\dagger \equiv (1/d)\int \phi dy$, which integrates the solid volume fraction ϕ through the depth, and the local volume fractions ϕ_0 in the shear layer [18]. In two-dimensional flows of spheres or disks, visualization can also reveal depth profiles of mean velocity u along the flow, fluctuation velocities, volume fraction and spin.

An important variable in all granular flows is the "granular temperature". In three dimensions, it is

$$T \equiv (1/3)\overline{u_i' u_i'}, \tag{12}$$

where u_i' is the fluctuation velocity along the direction i. Defined by analogy with the translational temperature of a hard-sphere gas, it is responsible for the viscous transport of momentum among grains interacting through brief collisions.

Numerical simulations produce more detailed information on velocities, temperature, volume fraction, and stresses [19, 20]. They reveal the role played by granular parameters like friction and normal restitution, and by the nature of the base and the lateral walls.

8.1 Flat, frictional base

On a flat, frictional base, flows of nearly spherical grains with depth $h \gtrsim 5d$ [19] feature a thin basal shear layer supporting a relatively passive denser overburden at relatively low inclination [18]. In the shear layer of thickness $\lesssim 2d$, grains roll appreciably around the vorticity $z-$axis, but frustrate each other's spin through collisions. There, the solid volume fraction ϕ_0 is smaller than in the overburden, and the granular temperature grows with $H^\dagger$ and α [18]. SFD flows occur in the range

$$\mu_I < \tan\alpha_{min} < \tan\alpha \leqslant \tan\alpha_{max} < \mu_S, \tag{13}$$

where μ_I is the friction in an impact of a single grain with the flat base, and $\alpha_S = \arctan\mu_S$ is the inclination at which a group of grains constrained in rotation begins to slide on a naked base. In the experiments of Louge and Keast with glass beads, $\mu_I \approx 0.14$, $\mu_S \approx 0.59$, $\alpha_{min} \approx 15.5^\circ$ and $\alpha_{max} \approx 20^\circ$.

For relatively shallow SFD flows, $H^\dagger \lesssim 5$, Louge and Keast observed a depth-averaged velocity $\overline{u}$ scaling as $h^{1/2}$ through a constant that increases with α [18]. Their results agreed qualitatively with those of Johnson, *et al* for $H^\dagger \lesssim 5$ in a facility with similar W/d [21]. In such shallow flows, side walls did not play a significant role [18].

Experiments with steady input exhibited recurring traffic waves consisting of upward-moving heaps fed from faster-moving grains upstream and reaccelerating downstream toward the SFD state. They also featured smaller "roll" waves moving downstream faster than the mean flow [18]. The waves betray inherent instabilities returning on a period

much longer than the mean shear rate. Because traffic waves inflate the flow depth significantly, they are affected by side walls. Their thickness also impedes measurements of h that are not instantaneous.

At greater depths, the data of Johnson, *et al* [21] bifurcated along two branches depending upon the method of supply. Occasional sharp transitions between these branches may be related to the traffic waves mentioned earlier. Side walls likely played a role in the momentum balance of the deeper branch with $H^{\dagger} \gtrsim 5$, as it does in the "super-stabilized heaps" described by Taberlet, et al. [22].

Walton observed SFD flows on a flat, frictional base [19] using MD simulations that are periodic in the $x-$ and $z-$directions at a value of $\tan\alpha \approx 0.31$ lower than the single, relatively large coefficient of friction $\mu = 0.4$ that he adopted for collisions with the base and among grains. He confirmed the dependence $\overline{u} \propto h^{1/2}$ and found that the shear layer grows thicker with increasing coefficient of restitution e, but that, surprisingly, $\overline{u}$ also decreases with e as a greater proportion of the flow experiences collisional dissipation. Because without side walls all forces between the grains and the base are exerted at discrete, small patches of contact, and because the average friction $[\mu_{eff} = \tan\alpha] < \mu$, contacts are not all slipping at the base in Walton's simulations, but instead have tangential forces F_t consistent with Coulomb's law $F_t \leqslant F_n$, where F_n is the force normal to the base. Because natural grains exhibit much smaller coefficients of friction in collisional impacts [23], it is unclear whether interactions with the base can be captured with a unique coefficient of sliding friction μ that is independent of the age or the relative velocity of the contact point [19], or whether a more subtle friction model is required [18].

Theories describing dense flows down flat, frictional inclines include the works of Savage [24], and Johnson, et al. [21], amongst others. Recently, by incorporating contributions from impulsive and enduring interactions with the base, Louge and Keast [18] proposed a theory producing quantitative predictions for the range of sustained flows observed in their experiments. They achieved closure of the theory using a balance between the production and dissipation of angular momentum in a narrow basal shear layer. In contrast to Johnson, et al. [21], they employed the balance of force normal to the flow to determine the normal component of the contact force.

8.2 Rough, rigid base

Dense SFD flows over rigid bases covered with bumps on the scale of order d exist at steeper inclinations than their counterparts on a flat, frictional plane and only above a minimum thickness h_{stop} that decreases with α such that $\lim_{\alpha \to \alpha_{min}} h_{stop} = \infty$ and $h_{stop}(\alpha_{max}) = 0$ [17]. Unless they are very thick ($h \gtrsim 10 h_{stop}$) [25] or previously accelerated to great speeds [26], they are mobilized through the depth [20], but generally exhibit a negligible mean velocity at the base. This complete mobilization results in $\overline{u} \propto h^{3/2}$.

They consist of three regions: a thin top "surface layer" where ϕ decreases abruptly toward the free surface; a "core" where ϕ is remarkably constant, but decreases with

increasing α; and a "basal layer" within a few grain diameters of the rigid bottom boundary where profiles of mean velocity u, granular temperature T, angular velocity ω and solid volume fraction ϕ depend on the nature of the base [27]. If the flow is sufficiently thick to establish a core, profiles in the latter are independent of the bottom boundary [28] with $T \propto (h-y)$, and $\omega = (1/2)du/dy \propto \sqrt{T}/d \propto (h-y)^{1/2}$. Thinner flows with $h \sim h_{stop}$ exhibit more complex profiles that depend on the nature of the bottom boundary, which generally dissipates fluctuation energy.

The MD simulations of Silbert, *et al* [20] further reveal that profiles are independent of e, while μ only affects the profile of u when $\mu \lesssim 1$, but it does not affect ϕ. This suggests that the value of ϕ in the core is independent of the dynamics of the flow.

Dense flows over a rigid rough base exhibit roll waves, but no traffic waves. These flows are affected by the presence of side walls [29], and thus are prone to degenerate into the "super-stabilized heaps" of Taberlet, et al. [22].

For flows down rough inclines, Louge [30] proposed a theory that models stresses as the superposition of a rate-dependent contribution arising from collisional interactions and a rate-independent part related to enduring frictional contacts among the grains. He showed that dense flows consist of the three regions ("basal layer", "core", "surface layer") mentioned earlier. He also distinguished basal flows with the smallest possible height, in which the core and surface layers have disappeared. Louge [30] derived simple closures of the governing equations for the three regions with insight from the numerical simulations of Silbert et al. [20] and the physical experiments of Pouliquen [17]. The theory captured the range of inclination angles at which steady, fully developed flows are observed, the corresponding shape of the mean and fluctuation velocity profiles, the dependence of the flow rate on inclination, flow height, interparticle friction, and normal restitution coefficient, and the dependence of the height of basal flows on inclination. The theory could also predict the flow behavior in terms of the parameter I introduced in section 5 [16].

9 The effect of interstitial fluid

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In many practically relevant particulate flows, the motion of the particles is intimately coupled with that of the interstitial fluid. For example, in beds of particles fluidized by a gas or a liquid, the drag force exerted by the fluid on the particles support their weight. This relative motion between the interstitial fluid and the particles gives rise to well known fluidization instability (e.g., see [31, 32]), leading to inhomogeneous structures that take the form of traveling voidage waves and bubbles in dense beds and clusters and streamers in dilute suspensions. Because of the importance of the relative motion in inducing these structures, these systems are commonly analyzed as two-phase flow problems. The same applies for dense phase and dilute phase pneumatic conveying.

There are many particulate flows where the presence of the interstitial gas is merely incidental and its motion is induced by the motion of particles. However, when the local-average velocities of the particles and the interstitial fluid are unequal, a net fluid-particle drag force results and this is also accompanied by a fluid phase pressure gradient. When this happens, the flow of the particles should be analyzed as a two-phase flow problem to obtain proper interpretation of the observed flow characteristics (e.g., see [33]). This effect becomes more and more pronounced as the particle size becomes smaller, and flows involving fine particles, where cohesive effects also become important, are frequently coupled to the interstitial fluid flow in a strong manner. The effect of interstitial gas on the rate of discharge of fine particles from hoppers and silos is well known [34, 35]. The interstitial gas is implicated in some of the particle flow characteristics observed in rotating drums (e.g., see [36]), and in the Brazil Nut and Reverse Brazil Nut effects in vibrated layers (e.g., see [37]). The influence exerted by the interstitial fluid in these examples is not driven by particle-particle cohesion or particle-boundary adhesion, and they can occur even in cohesionless systems.

9.1 Some physical issues

Homogeneous fluidized suspensions of uniformly sized, cohesionless particles fluidized by a gas are always unstable [38] and tensile strength of particle assemblies resulting from cohesion is important for explaining the window of stable bed expansion observed for Geldart Group A particles. As the strength of cohesive interaction is increased (for example, by decreasing the particle size), the hierarchy of inhomogeneous structures observed in fluidized suspensions changes appreciably, but this change is not well understood.

Fluidization of uniformly sized particles is possible only over a modest range of cohesive interactions – typically for $Bo <\sim 10$, where Bo (Bond number) is the ratio of the maximum cohesive force between particles and the particle weight – and for $Bo >\sim 10$ fluidization can be achieved only if the gas flow is supplemented with some means such as vibration [39, 40, 41, 42] to break up the agglomerates. While it is easy to understand that one is simply fluidizing agglomerates in vibrofluidized beds of cohesive particles, quantitative predictions of the effects of vibration and fluidization on the distribution of agglomerate sizes are not yet available. The agglomeration and breakup dynamics in these systems, which is important in mixing devices, is even less understood. Vibration can also affect the stability of fluidized beds [43].

Irrespective of whether the interstitial gas plays an important role or not, cohesion between particles affects the dynamics of particulate flows appreciably. For example, weakly cohesive systems manifest stick-slip flows in the shear layer in cylindrical tumblers – the alternating slow creep and rapid slip contributes to enhanced mixing [44]. Thus, by tailoring cohesion, one can enhance mixing or mitigate tendency to demix in particle handling devices. A better understanding of the stick-slip flow at the particle level and its effect on the mesoscale and macroscale flow and mixing can lead to more efficient mixing devices.

9.2 Some modeling issues

The nature of the model employed depends on the scale of enquiry. Microscopic analysis probing the detailed motion at the level of the individual particles aimed at developing closure for coarser analysis of flow is generally based on the Navier-Stokes equations for the fluid and the Newtons equations for the linear and angular momenta of the particles (e.g., see [45]). This type of modeling is particularly useful to develop better closure relations for fluid-particle drag force. In most practical systems involving fine particles and gas as the interstitial fluid, the Reynolds number associated with the relative motion between the fluid and the particles is invariably small. The drag coefficient then depends only on the particle volume fraction, particle size (and distribution, if applicable), and some metric of the particle configurations (such as the radial distribution function). As cohesive interaction between particles can be expected to influence the microstructure of the particle assemblies, there may be a systematic effect of the strength of cohesion (e.g., relative to gravity) on the drag coefficient. Some exploration of this effect, leading to refined drag laws, is worthwhile.

At a somewhat coarser (mesoscopic) level, especially for gas-particle systems, the gas phase is treated in a local-average sense while the particle motion is evolved through DEM simulations (e.g., see [46, 47, 48, 49]) – this approach has been used to examine the influence of cohesion between particles on fluidization-defluidization characteristics. As noted earlier in section 6.1, only a small number of particles (typically less than a million) can realistically be simulated through DEM simulations and hence the main role of this class of simulations has been to develop a better physical understanding of the flows and closures for an even coarser scale analysis.

In most problems of practical interest, the number of particles involved is very large (tens to hundreds of million), and hence, solving for the motion of each and every particle in the assembly is computationally expensive and unaffordable. This consideration has driven the development of continuum models through ensemble-averaging of the equations governing the motion of the individual particles as a practical alternative to probe macroscopic flow characteristics. In this approach, the particle phase is treated as a continuum and locally-averaged quantities, such as the volume fraction, mean velocity and mean-squared fluctuating velocity of the particle phase, appear as dependent variables (e.g., see [50, 31]). The averaging process erases the details of flow at the level of individual particles; but their consequences appear in the averaged equations through terms for which one must develop closure relations (a.k.a. constitutive models). Derivation of the general form of the averaged equations and associated constitutive models has been the subject of much research, but such theories are invariably limited to a small subset of cases of practical importance. For example, most of the analysis is limited to cohesionless and uniformly sized particles.

The bulk of the analysis of flows via two-fluid models published in the literature handle particle phase stress through the application of critical state theory (developed in soil

mechanics) for quasi-statics flows, the kinetic theory of granular materials for rapid granular flows or simply some *ad hoc* expressions. How to bridge the quasi-static and rapid granular flow regimes (see Fig. 4 discussed in section 3) is an important frontier. The transitional region connecting the quasi-static regime has been examined through experiments and continuum modeling by Tardos et al. [51] who build on an earlier paper by Savage [52], and through DEM simulations of cohesionless particles by Campbell [53]. A systematic study of the influence of cohesion between particles on the rheological characteristics in the various regimes of flow is much needed, and this is an area where DEM simulations can be used to develop a better physical understanding of force chains and structures at difference length and time scales. These can then lead to better closures for continuum model for flows of cohesive particles.

There are at least three major limitations in using continuum models for particulate flows and the more general two-phase flows:

1. In many flows involving dense assemblies – irrespective of whether the constituent particles are cohesive or cohesionless – there are regions where the assembly behaves as a rigid body and others where the particles do flow (e.g., funnel flow through hoppers and dense phase conveying). Such mixed flows are not well described by todays continuum models.

2. When cohesion is important, there is a strong history dependence (discussed in section 3; also see e.g., [54]), and rheological models to capture such history effect remain to be developed.

3. Most gas-particle flows are unstable and they manifest inhomogeneous structures on a wide range of time and length scales. There is often no clear separation of scales – for example, force chains in quasi-static flows of dense assemblies may extend over macroscopic length scales – and the fluctuations in locally averaged quantities can be vary large (e.g., see [55]). Thus, in many cases, the spatial/temporal resolution at which the commonly used closures for the continuum models are valid is not at all clear.

Research aimed at improving our understanding of these issues would be very useful in advancing our ability to model flows in large scale systems.

Some authors argue that even the continuum models should be further coarse-grained to get practically useful models (e.g., see [56, 57, 55, 58]). Such coarse-graining will change the effective drag force and stress closures. For example, McKeen and Pugsley [59] found that their two-fluid model simulations of fluidized beds of FCC particles were able to capture the experimental data if they assumed an apparent particle size which is larger than the true particle size; because of the weakly cohesive nature of the FCC particles, it is conceivable that one is really fluidizing agglomerates of particles and that the closures should be based on the agglomerate size. This then leads us back to the question as to how one can predict the effective agglomerate size.

Summarizing the discussion of this section, we pose the following list of challenges, which should be tackled:

1. Develop criteria to expose when the interstitial fluid flow is important in a given problem involving powder flow.

2. Develop a physical understanding of the effect of interparticle forces on the hierarchy of flow-induced inhomogeneous structures.

3. Develop quantitative models for the effects of vibration and pressure pulsations generated through a microphone – either by themselves or in conjunction with fluidizing gas flow – on the dynamics of particle agglomerates.

4. Develop a better understanding of stick-slip motion of cohesive powders and how it can be manipulated to get optimum flow and mixing characteristics.

5. Probe the possible effect of cohesion on the drag coefficient, through its influence on the microstructure of the assembly.

6. Through a combination of experiments and DEM simulations, develop better continuum rheological models for assemblies of cohesive particles – all the way from quasi-static to rapid flow regimes, bringing in the path- and history- dependence manifested by cohesive systems and the compressibility effect discussed in section 3.

7. Develop equations of motion and associated closures by coarse-graining over mesoscale structures (such as collections of agglomerates).

10 Recommended research challenges in granular and granular-fluid flows

Granular and granular-fluid flows pose challenges of wide interest to Physics, Applied Mathematics, Civil Engineering, Chemical Engineering, Materials Science, Mining, and Geophysics. Our report highlighted the main issues in powder flows.

We also produced the following statement that the National Science Foundation may wish to adopt to solicit proposals on this subject. IFPRI's hope is that the adoption of this document for publication on the NSF web site will encourage scientists to engage in research of interest to the IFPRI membership.

10.1 Recommended NSF statement

"In an effort to address issues of broad interest to the chemical, pharmaceutical, civil and mining industries, as well as to geophysical sciences, the National Science Foundation (NSF) encourages fundamental research on granular and granular-fluid flows.

Such flows include dispersed solids at relatively high volume concentrations, with or without appreciable influence of the interstitial fluid phase. Granular flow characteristics invariably span multiple time and length scales. On the microscopic level, particles may be affected by non-linear and non-local interaction mechanisms, such as ephemeral collisions or fluid drag. They may also experience long-range force chains connecting mesoscopic flow regions. Their volume fraction, stress, and energy typically fluctuate spatially and temporally with amplitudes comparable to the mean. The micro- and meso- scale dynamics may lead to instabilities resulting in coherent structures and inhomogeneous flows at the macro-scale. Their interaction with boundaries is often complex and poorly understood.

In this context, the NSF seeks cross-disciplinary research combining at least two of the following three approaches: experimental, numerical and theoretical.

By recording flow variables such as volume fraction, velocity, or stress, experiments can test the validity of numerical simulations or the predictions of theory. They can also result in the discovery of new science or in the creation of novel diagnostic techniques.

Direct numerical simulations are meant to reproduce the behavior of discrete particles or elements of fluid. By measuring flow variables in regions that are inaccessible to experiments, simulations can inform the development of theory, for example in the derivation of constitutive relations. Numerical algorithms should be grounded in physics by featuring independently measurable material and fluid properties, rather than merely appearing to capture the correct phenomena.

Because granular and granular-fluid flows may not exhibit a clear separation among the spatial and temporal micro-, meso- and macro- scales, advanced multi-scale theories may be needed to analyze them. Theories should also produce governing equations and boundary conditions suitable for predicting systems too large for discrete numerical simulations.

While the NSF seeks elucidation of fundamental paradigms involving, for example, monodisperse spheres or Newtonian fluids, it also encourages consideration of at least one other challenge, such as friction, effects of polydispersity and size, bulk compressibility, particle cohesion (e.g., due to liquid bridges and/or interparticle surface forces) or repulsion (e.g. due to electrostatic forces), viscous and/or lubrication effects in a three-phase system, or phase transitions. While the research may be relevant to process applications, its primary objective must be to generate fundamental physical insight."

11 Conclusions and Forward Look

In this report, we summarized salient questions on interparticle forces, bulk behavior, constitutive relations, scaling relations, and numerical modeling in powder flows. We closed by discussing the example of dense inclined flows of monodisperse spherical particles to illustrate a situation for which the physics is simple enough to reconcile experiments, numerical simulations and theory.

The report reflected the diversity of expertise and interests in the group. Clearly, it put

forth more questions than it answered. In this context, we suggested a strategy for further research in powder flows, which the NSF is encouraged to adopt. Our hope is that the resulting work will benefit the IFPRI membership by leveraging its resources into research that academics could explore in future.

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