Modelling powder flow through screw feeders

Proposal submitted to IFPRI by
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Summary: This proposal outlines a study aimed at developing a theoretical model for understanding and predicting flow in twin screw feeders, with the aim of linking feeder performance to the powder properties, feeder geometry and dimensions, and operating conditions. We aim to start with non-cohesive powders, and progressively build in cohesion and other features to address industrially relevant powders. The predictions of the model will be tested against experimental measurements of the mean flow rate, the stress and bulk density at the casing measured by flush mounted sensors, and the velocity profile at the free surface measured by video imaging. DEM simulations will be used to validate and refine the theoretical studies, and guide experimental measurements.

1 Background

To my knowledge, no previous study has conducted a detailed theoretical analysis of the flow of powders in screw feeders using a continuum mechanical model. The reason for this is that constitutive models for powder flow are still in the stage of development, and model validation is typically attempted in simple shear flows, where the problem solution and experimental validation are easier. The flow in screw feeders is complex and three-dimensional, and developing an undertanding is as much a challenging scientific problem as it is of practical importance to industry. Despite the challenges, I believe my group is in a position to make a concerted attempt at tackling the problem, as we have experience in understanding reasonably complex flows. Section §1.1 describes some of our recent work, illustrating how a synergistic combination of theory, experiments and DEM simulations has helped us gain a fundamental understanding of an important aspect of non-cohesive powder flow, and resulted in the formulation of a new constitutive model. The features of this model, which we will use in this study, are then explained in §1.2.

1.1 Our recent work: A puzzling phenomenon in powder rheology, its resolution, and a theoretical understanding.

Motivated by predictions of one of our earlier theories for dense, slow flow of powders [1], we conducted experimental rheometry of non-cohesive powders [2, 3], wherein a custom-built cylindrical Couette device and sensitive 3-axis force sensors were used to measure the stress as a function of position along the outer cylinder (Fig. 1a). We made the surprising observation that when the powder is sheared, the vertical shear stress σ_{rz} at the outer cylinder changes sign, and the radial normal stress rises exponentially with depth (Fig. 1b). The findings were puzzling because they are contrary to previous measurements [4] and the predictions of plastic and visco-plastic theories [1, 3], which show a liquid-like linear rise of the normal stress with depth. To investigate this further, we used a combination of DEM simulations and high-speed video imaging of the free surface [5] and uncovered a remarkable secondary flow, in the form of a single toroidal vortex that spans the entire Couette cell and whose sense is anti-centrifugal. Further, we showed that the vortex is driven

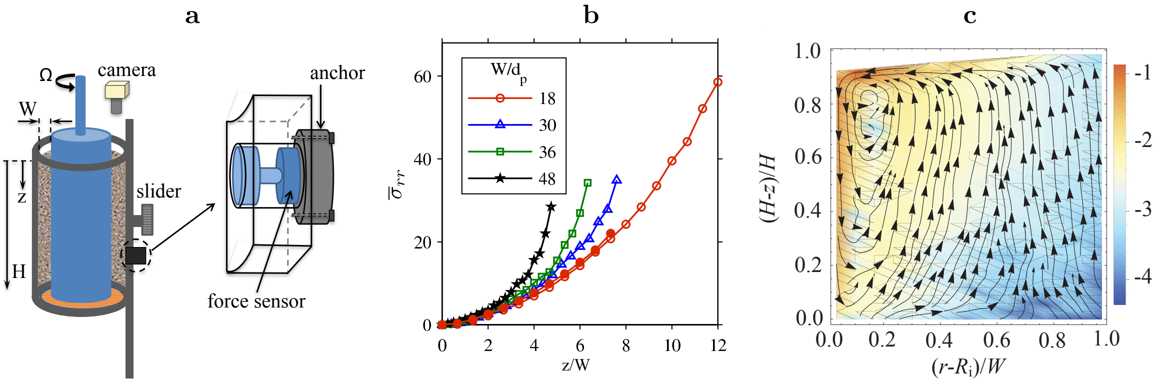

Figure 1: (a) Schematic figure of our instrumented cylindrical Couette apparatus. (b) The radial normal stress on the outer cylinder (scaled by $\rho g W$) for glass beads of mean diameter $d_p \approx 0.83$ mm as a function of the depth for different Couette gaps (from Ref. [2]). (c) The secondary flow in a vertical cross section of the Couette device – the streamlines represent the velocity vector in the cross section, and the colors indicate the magnitude of $\log(v_r^2 + v_z^2)^{1/2}$ (from Ref. [5]).

by shear-induced dilation. Using a simple plasticity model, we showed that the secondary flow explains the puzzling of the stress anomaly. This study underlines the importance of the coupling between density and flow, as it shows that dilatancy, which was thought to be relevant only in thin shear layers and ignored in continuum models, drives a macroscopic secondary flow that has a large rheological signature. This led us to propose a non-local constitutive model that incorporates dilatancy – the features of the model are described in §1.2.

1.2 Theoretical model

Continuum theories for granular flows enforce the balances of mass and momentum,

$$\mathrm{D}\rho/\mathrm{D}t = -\phi \boldsymbol{\nabla \cdot v}, \quad \mathrm{D}\boldsymbol{v}/\mathrm{D}t = \boldsymbol{\nabla \cdot \sigma} + \rho \boldsymbol{g} \tag{1a, b}$$

where $\mathrm{D}/\mathrm{D}t$ represents the material derivative, ρ is the density, $\boldsymbol{v}$ the velocity vector, $\boldsymbol{\sigma}$ the stress tensor and $\boldsymbol{g}$ is the gravitational body force. For closure, a constitutive model for $\boldsymbol{\sigma}$ is needed; the commonly used model for the regime of slow flow is that of classical plasticity [6, 7], comprising a yield condition that specifies the states of stress for which plastic flow can occur, and a flow rule that relates the components of the strain rate and stress tensors. The choice of a simple yield condition and flow rule leads to the constitutive relation [7]

$$\boldsymbol{\sigma} = -p\,\boldsymbol{I} + \frac{2\mu\, p_\mathrm{c}(\phi)}{\dot{\gamma}}\,\boldsymbol{D}, \quad p = p_\mathrm{c}(\phi)(1 - \frac{\mu_\mathrm{b}}{\dot{\gamma}}\,\boldsymbol{\nabla \cdot v}). \tag{2a, b}$$

Here p is the pressure, ϕ is the powder volume fraction, $\boldsymbol{D}$ is the strain rate tensor whose scalar magnitude is $\dot{\gamma} \equiv (2D_{ij}D_{ji})^{1/2}$, and $p_\mathrm{c}(\phi)$ is the pressure at the *critical state* of isochoric deformation [6]. The model parameters are the Coulomb friction coefficient μ and the bulk plastic modulus μ_b. This model has been used in several studies [8–10], but it suffers from three crucial deficiencies: (a) the velocity profile in simple shear flows is indeterminate; (b) it does not predict dilation (or compaction) at constant pressure, which was shown to be important in §1.1; (c) for time-dependent flows, the model results in a mathematically ill-posed problem [11].

We have recently proposed a non-local model [12] that overcomes all the deficiencies of classical plasticity, and is superior in significant ways to other non-local models proposed in recent years [1, 13]. Our model is based on the simple idea that the strain rate and density at one spatial location are caused not only by yielding at that point, but in a small region around it. This idea reflects inhomogeneities observed in experiments, such as force chains, and correlated motion of groups of grains. The resulting constitutive relation is

$$\boldsymbol{\sigma} = -p\,\boldsymbol{\delta} + \frac{2\mu\,p_{\mathrm{c}}(\phi)}{\dot{\gamma}}\,(\boldsymbol{D} - \ell^2\,\nabla^2\boldsymbol{D}), \tag{3a}$$

$$p = p_{\mathrm{c}}(\phi)[1 - \frac{\mu_{\mathrm{b}}}{\dot{\gamma}}(\boldsymbol{\nabla}\cdot\boldsymbol{v} - \ell^2\,\nabla^2\boldsymbol{\nabla}\cdot\boldsymbol{v})] - \ell^2\,\frac{\mathrm{d}p_{\mathrm{c}}}{\mathrm{d}\phi}\,\nabla^2\phi. \tag{3b}$$

Here, the terms multiplied by ℓ^2 (highlighted in red) are the non-local terms, with ℓ being the mesoscopic length scale that characterizes non-locality. It is clear from (3b) that the volume fraction ϕ can vary even when the pressure is constant, which is indeed commonly observed in the form of dilation in shear layers. Equation (3) is the constitutive model we will be using in the initial part of our investigation on non-cohesive powders; we will subsequently incorporate the effects of cohesion.

2 Proposed programme

The early application of continuum models for screw feeders [14] considered the idealized condition of perfect slip at the screw and casing surfaces, and the slope of the free surface determined from the static balance of forces between friction at the screw surface and gravity. Recent studies using DEM simulations [15] have found that the actual flow rate differs significantly from the idealized estimate, largely due to the complexity of the flow arising from the shear forces on the powder imparted by the screw(s) and casing. Therefore, to derive more realistic estimates of feed rates, and relate them to the feeder geometry and powder properties, detailed modelling of the flow, guided by DEM simulations and validated by experiments, are essential. The description of our recent work in §1.1 and §1.2 would hopefully have made the case that we are well placed to carry out this study. An outline of the proposed work under each of the elements is given below, followed by brief descriptions of the specific elements of our study in §2.2.

2.1 Outline of proposed work

Theoretical modelling
I propose to begin the modelling effort by first considering non-cohesive powders. Firstly, the exercise of posing the problem mathematically will give us useful heuristics for the feed rate as a function of the various dimensionless parameters that arise, whose influence can be tested systematically in the experiments. For the detailed numerical solution of the governing equations, the complexity of the geometry suggests that it is prudent to approach the problem in steps, going from a simple geometry that mimics some important features of a screw feeder (Fig. 2c) and finally reaching the time dependent flow in the full domain (Fig. 2a,b). There are also other challenges to be overcome in our modelling effort, such as choosing physically reasonable boundary conditions. The second phase of our modelling efforts will concentrate on incorporating cohesion in the constitutive model. The extension will require more than simply modifying the yield condition, as is often done – we must consider how cohesion alters the flow rule, and thereby the kinematics in the

shearing regions. Details on each of these aspects are given in §2.2 below.

Experiments
We will attempt to make measurements of the gross feed rate as a function of material properties and geometric parameters. Moreover, we will make detailed measurements of the stress and density at the casing as a function of axial position, and the velocity on the free surface of the powder bed. These studies will useful not just for validating our model, but also suggest ways in which the model may be refined, particularly for cohesive and aeratable powders.

DEM simulations
Apart from validation of the stepwise approach of our theoretical modelling, we expect DEM to provide information on the flow in the bulk that is difficult to obtain from experiments. Unlike the solution of the theoretical model, the complexity of the geometry poses no serious difficulty for DEM. The simulations will be particularly useful in model formulation and refinement for cohesive powders, for which constitutive models remain poorly developed.

2.2 Specific elements of the proposed investigation

A. Identification of dimensionless groups and heuristic analysis for feeder performance: The first outcome of posing the problem mathematically is that the relevant dimensionless groups that control feeder performance will become apparent. The idealized analysis of Ref. [14], discussed earlier, gave the volumetric feed rate in a single screw feeder as $\alpha A \Omega p$, where A is the cross section area of the feeder, Ω the frequency of screw rotation, and p their pitch (Fig. 2b). The 'efficiency factor' α depends on the angle of inclination of the screw surface to the radial line and the coefficient of wall friction μ_w of the screw feeder. For a twin screw feeder in a more realistic scenario, we expect shear of the powder, the slip coefficient K at boundaries (see item B below), the degree of intermeshing of the screws, powder friction coefficient μ and cohesion stress σ_{coh} (see item D below) to determine feeder performance, thereby giving rise to additional dimensionless parameters, such as μ/μ_w, $\sigma_{\text{coh}}/(\rho g D)$, K, etc. that α will depend on. This will now allow us to conduct a sensitivity analysis by experiment and DEM, and thereby determine the controlling parameters that determine the feed rate.

B. Detailed modelling of the flow of non-cohesive powders: Substituting the relation for the stress tensor $\boldsymbol{\sigma}$ from (3) into the momentum balance (1)b, we get a system of partial differential equations of fourth order in $\boldsymbol{v}$ and third order in ϕ. Solution of the equations requires sufficient boundary conditions for the velocity and volume fraction in each direction than for classical plasticity. The lack of physically realistic boundary conditions has been a lacuna in modelling of powder flow: for example, the majority of studies assume no-slip, while there is clear experimental evidence of slip. In our earlier studies [1, 12], we have used the boundary conditions

$$\boldsymbol{u} - \boldsymbol{u}_w = -K d_{\text{p}}\, \boldsymbol{n} \times \boldsymbol{\omega}, \quad \boldsymbol{n}\cdot\boldsymbol{\sigma}\cdot\boldsymbol{t} = \mu_w\, \boldsymbol{n}\cdot\boldsymbol{\sigma}\cdot\boldsymbol{n}, \quad \boldsymbol{n}\cdot\nabla\phi/\phi = \boldsymbol{n}\cdot\nabla\boldsymbol{v}\cdot\boldsymbol{t}/\boldsymbol{v}\cdot\boldsymbol{t} \quad (4\text{a, b, c})$$

where $\boldsymbol{n}$ and $\boldsymbol{t}$ are the unit normal and tangent vectors to the boundary. Above, (4a) determines the slip velocity, with K being the slip coefficient and $\boldsymbol{\omega}$ the powder vorticity, (4b) specifies that the ratio of the shear and normal stresses for plastic yield, and (4c) specifies the volume fraction at the boundary. These boundary

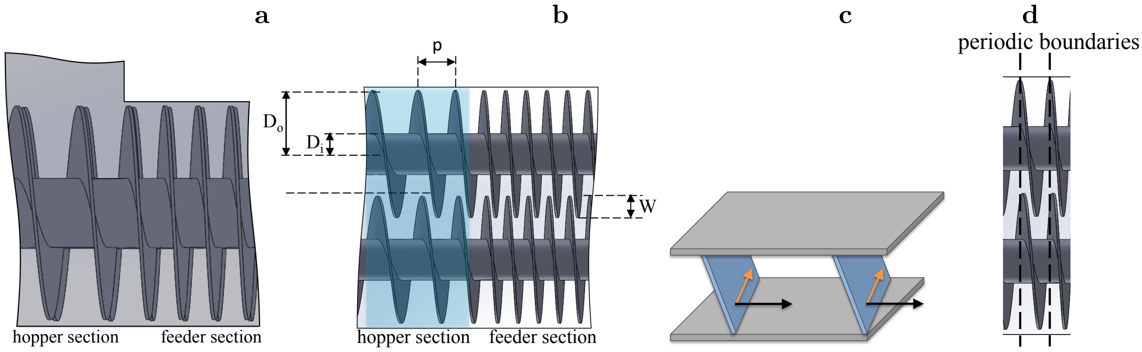

Figure 2: (a, b) The side and top views of the full domain, including the hopper and feeder sections. (c) Simplified rectangular mimic of the screw feeder. The two planar 'scrapers' (blue), which simulate the screw have constant velocity components in the axial and lateral directions. (d) The domain of width equal to one pitch of the screw with periodic boundaries on the left and right boundaries (dashed lines).

conditions make good qualitative predictions for flow in a split-bottom Couette device [12], but their validation by DEM simulations and experiment in other flows is necessary.

The governing equations will be solved numerically by discretizing the spatial domain using the finite volume method. Before solving the full time-dependent problem that includes the hopper and feeder sections (Fig. 2a,b), it is prudent to proceed in steps, and test the computations against DEM simulations at each step. The first step, shown schematically in Fig. 2c, is to simulate a simplified rectangular mimic of the helical screw – the screw is replaced by planar 'scrapers' that are inclined to the top and bottom walls, and have velocity components in the axial and lateral directions. Despite the simplification, the flow in the cross section will be non-trivial, and we expect this exercise to not only provide confidence in our theoretical model, but also provide insight into the swirling flow generated by the screws.

The next step will be to solve for the flow in the 'fully developed' feeder region by considering a domain of width equal to one screw pitch (Fig. 2d), with periodic boundary conditions applied at the left and right boundaries. Particular attention will be paid to understanding the flow in the intermeshing region between the two screws, as it will provide useful information on the enhanced effectiveness of twin screw over single screw feeders. We will finally consider the time-dependent problem over the full domain, including the hopper and feeder regions, wherein the time variation in the feed rate do to imposed variations in the hooper flow (such as refill events) can be explored. The time-dependent analysis will also be useful in designing a realtime feed-back control protocol for the feed rate.

C. DEM simulations We propose to use the open source LAMMPS and LIGGHTS packages for our simulations; the latter allows the user to insert a complex moving surface into the flow domain. This significantly eases the handling of the complex screw geometry, allowing us to concentrate on the physics of particle-particle and particle-wall interactions that determine feeder performance. The DEM simulations will be used for validating of the predictions of our theoretical model in each of the steps mentioned in item B above, and along with the experiments, suggest refinements and course corrections in the modelling.

Perhaps the most important utility of DEM will be in providing insight into

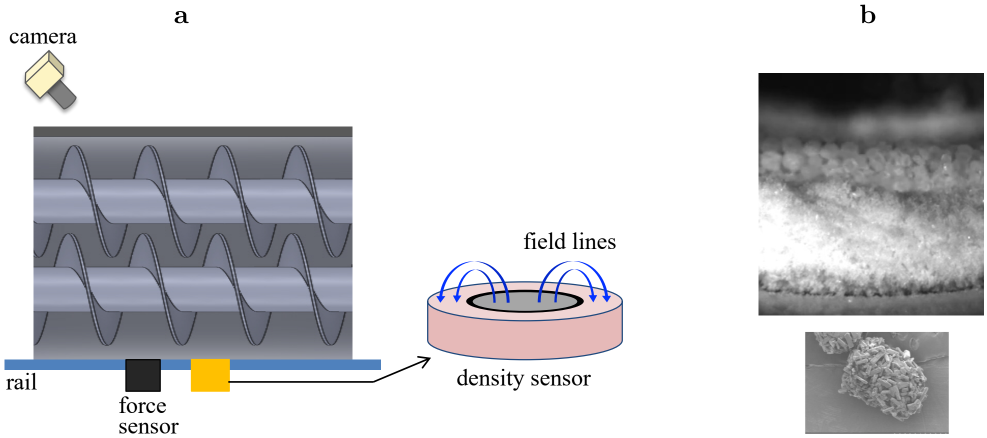

Figure 3: (a) Schematic of the proposed experimental apparatus, with stress and density measurements at the casing of the screw feeder. The sensors will be mounted on a sliding rail, and the force sensor and mounting will be similar to Fig. 1a. The density sensor will be a coaxial electrode capacitance/inductance sensor. The velocity field on the free surface of the powder will be measured by vide imaging. (b) Observation that the formation of particle agglomerates enhances shear of cohesive powders. The top panel shows the free surface of a powder sheared in our Couette device, where the formation of agglomerates near the rotating inner cylinder is apparent. The bottom panel is an SEM image of an agglomerate.

modelling cohesive and aeratable powders, discussed in item E below. We propose to use simple models for particle cohesion in DEM (e.g. van der Waal attraction, liquid bridge cohesion) and understand how cohesion alters the wall stress, flow and density fields. This information will help us build models for cohesive powders, and also inform how the experiments should be tailored to answer questions on how cohesion affects feeder performance.

D. Experiments We will measure as a function of time the feed rate by monitoring the weight of material at the exit vessel, the stress and density on the casing as a function of axial position using flush-mounted force and capacitance/inductance sensors, and the velocity at the free surface of the powder by video imaging, as shown in Fig. 3a. From these measurements, we will extract the mean quantities and their fluctuations. The latter will be important in assessing the variability of feeder performance for different materials and feeder geometries, and also in assessing how variations in the inlet conditions alter the flow rate at the exit of the feeder. We hope to determine the optimal design of the feeder that will buffer the exit flow rate against variations in the inlet conditions. Most importantly, all our measurements will be used to validate the theoretical predictions, described in item A and B above. As already mentioned, we expect that the DEM simulations to help us refine our experimental protocol and measurements, and help ask the right questions.

E. Extending the theoretical model to cohesive and aeratable powders Though listed last, this is an aspect we will start thinking about from the very beginning, as it is the most challenging aspect of the proposal. The conventional method for incorporating cohesion is to add a tensile component σ_{coh} to the pressure, i.e. by replacing the pressure p in (2a) and (3a) by $p - \sigma_{\text{coh}}$. While this does increase the threshold shear stress for plastic yield, it does not alter the kinematics. The kinematics is determined by the flow rule, the simplest (and commonly used) form of which is $D'_{ij} = \dot{\lambda}\, \sigma'_{ij}$, where $\dot{\lambda}$ is termed the 'fluidity', and the primes on the stress and strain rate components indicate that they are the deviatoric parts. For non-cohesive powders, it can be shown that $\dot{\lambda} = -\dot{\gamma}/p_c(\phi)$ [7], which was used to derive the constitutive relations (2) and (3). For cohesive powders, $\dot{\lambda}$ must be a function of σ_{coh} – while we have some preliminary ideas on how this could be incorporated, we await careful DEM simulations and imaging experiments to provide a clearer picture.

One aspect of cohesive powders that we have observed in some recent experiments is the native powder does not shear initially (but just slips at the moving wall), but with time the formation of agglomerates enhances the fluidity, after which the material shears almost like a non-cohesive powder – this is illustrated in Fig. 3b. This suggests that an evolution equation for agglomerate formation must also be included in the theoretical model, and that the fluidity must depend on the volume fraction of agglomerates. This will be an aspect that we will look into, and here again we will rely on careful imaging experiments and DEM simulations to guide model development.

In aeratable powders, the particles are fine enough that air drag make a significant contribution to the force balance on the particles. In the theoretical model, the equations of motion must be supplemented by the those for the gas, with a drag force linking the two. Such models have been widely used to study fluidization of powders, and reasonably accurate correlations for the drag are available in the literature. Hence, we do not see this as a significant challenge.

2.3 Critical unknowns that may affect programme outcome or direction

Most of the critical unknowns relate to cohesive powders: for theoretical modelling, the question is how the constitutive model for the stress (3) should be modified to model the effects of cohesion in a physically realistic manner. For DEM simulations, the question is what form of the cohesive force is representative of the interaction of powders that are important to industry. We are hopeful that the synergistic combination of theory, DEM simulations and experiments will answer these questions, but we will very much benefit from the experience and knowledge of domain experts in IFPRI.

There are some relatively minor unknowns that may affect the course of the programme, such as the numerical method used to solve the governing equations in §2.2B. There are instances when the finite volume method is numerically unstable, and if we encounter this we will have to use another numerical method. However, I am confident that our step-wise approach will identify and solve these problems early in the programme.

2.4 Expected year-wise accomplishments (with reference to itemized list in §2.2)

Year 1: Item A would be completed; the first step of item B, namely the rectangular mimic would be underway; item C for the rectangular mimic and the fully developed feeder section would be completed. Building the apparatus for item D would be underway. Some efforts in item E would have been initiated.

Year 2: The second step of item B, namely the fully developed feeder section is expected to be completed, and the third step (time dependent solution of the full domain) initiated. Work under item C for cohesive powders would be ongoing.

Under item D, experiments of model non-cohesive and cohesive powders would be ongoing. The first attempt at modelling of cohesive powders in item E would be initiated.
Year 3: Items B, C and D are expected to be completed. Under E, it is expected that some candidate constitutive models for cohesive powders would have been formulated, and numerical computations of the theoretical model would be completed. Comparison of the results of theory, DEM simulations, and experiments (under items B, C, D and E) would be concluded.

2.5 Leveraging current programmes in my research group for the project

As explained in §1.1, I have an active ongoing programme on the rheology of dense powders – I expect this project to be a nice extension of our current work. My group has also initiated a programme on characterization of the rheology and 'flowability' of cohesive powders. Application of our experience in theoretical modelling to the twin screw feeder will be challenging, but also satisfying due to its practical relevance to industry.

2.6 Support from IFPRI members

Support from IFPRI members would come in useful in the following ways:
1) Provide model powders of industrial relevance for which precision feeding is important.
2) Provide samples of "brittle, ductile, and elastoplastic" materials mentioned in the project brief, which we could characterize rheologically.
3) Access to feeders of different scales and design would be very welcome.
4) We would appreciate receiving data logged during screw feeding of "difficult" powders, if available, for comparison with our experimental data on model powders.

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