Forces on the walls and stagnation zones in a hopper filled with granular material

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Abstract

We measure the pressure and the shear forces acting on the walls of an outflowing hopper using Molecular Dynamics simulations. We find very strong fluctuations which for large opening angles follow a power spectrum but have white noise for smaller angles. We also calculate the shape of the stagnation zones that appear during funnel flow and compare it to the experimentally observed ones.

The outflow of granular materials from hoppers and silos is an important technological problem although it seems to be so commonplace and low-tech. After many years of uninterrupted service a silo might one day suddenly succumb under a “siloque” or similar shock phenomena of surprising violence causing considerable harm. In fact silos and similar recipients are by orders of magnitude the industrial structures most susceptible to collapse. The reason for these catastrophic events are that the forces that the flowing granular material exerts against the wall of the container can fluctuate by many orders in magnitude.

In fact, granular media are capricious systems – very badly understood from the theoretical point of view. Their flow behaviour presents many astonishing anomalies [1–3], among them enormous, spontaneously triggered density fluctuations which are at the origin of the strong pressure variations on the container walls. These fluctuations have been studied experimentally. Using X-rays Baxter et al. [4] visualized wave-like patterns emanating from the outlet of a two dimensional wedge-shaped hopper. Also previous authors [5–7] had observed the formation of similar structures. Brown and Richards [8] explained the density fluctuations during the outflow with non-random dilatant waves but their experiments with a single layer had limitations due to irregular sticking to
the plate. Similarly rather erratic shock-like density waves have been observed in flow through pipes [9] and down inclined planes [10]. Another experimentally observed ubiquitous phenomenon in granular media seems to be $1/f^\alpha$ noise. Lui and Jaeger [11] recently measured the acceleration of a particle inside a bulk of glass beads that were excited by a small amplitude vibration. Its Fourier spectrum in time showed power law decay over many orders of magnitude.

Baxter et al. [12] also measured the stresses acting on the walls of a three dimensional hopper with an opening angle of 45° during the outflow of sand. They observed a power law decay in the spectrum of the time dependence of the normal stress (pressure) where the exponent strongly depended on the run.

Recently substantial progress has been made in understanding the ubiquitous phenomenon of strong fluctuations forming in a self-organized way in systems of inelastically colliding particles [13] as they are also observed in earthquakes [14] or traffic jams [15]. The formation of these erratic density and force fluctuations is intimately related to the ability of granular materials to form a hybrid state between a fluid and a solid: When the density exceeds a critical value which some authors call the critical dilatancy [16,17], granular materials resist to shear like solids. In regions, where the density is below this value they will behave almost like fluids, like in an hourglass or on a vibrating plate. In the presence of density fluctuations the rheology can therefore become rather complex.

Two microscopic facts seem to be responsible for the strong density fluctuations: On one hand one has in granular media solid friction between the grains. This means that when particles are pushed against each other a finite force is needed to start or maintain a relative tangential motion between them giving rise to arching, i.e. the formation of stress-free zones below bridges, and a complex contact network that transmits the stresses. On the other hand a granular material is internally disordered, giving a natural source of noise.

Various attempts have been made to formalize and quantify the complicated rheology of granular media. Continuum equations of motion [18] have been proposed and within this context a stability analysis showed clustering due to dissipation [19] and a flux-density relation implying the existence of kinematic waves [20]. Some very encouraging results have been obtained for the spontaneous appearance of density fluctuations and waves in pipe flow using a cellular automaton [21] and a Lattice Boltzmann model [22]. This is why we chose to study these phenomena using Molecular Dynamics (MD) simulations of inelastic particles with static and dynamic friction in two dimensional systems. In fact, MD simulations [23] have already been applied to granular media to model outflow from a hopper [24–26], shear flow [27], convection [28] and segregation [29] on vibrating plates, avalanches on a sand pile [30], flow through a pipe [9] and others. In particular the power spectrum of the density flow in two dimensional hoppers has been calculated in Ref. [31] and it was found to follow a power law with an exponent of up to $\alpha = 2.6$ over more than two orders of magnitude.

We consider a system of $N$ spherical particles of equal density and with diameters $d$ either all equal or chosen randomly from a Gaussian distribution of width $w$ around
$d_0 = 1\text{ mm}$. These particles are placed into a hopper of size $10 \times 40\text{ cm}$ with the orifice at a height of $20\text{ cm}$ and a diameter of $D = 2\text{ cm}$. The angle with the horizontal, $\Theta$, can be varied (for definition see Fig. 1b). To calculate the experimentally more commonly used opening angle one simply has to subtract two times our angle $\Theta$ from $180^\circ$.

When two particles $i$ and $j$ overlap (i.e. when their distance is smaller than the sum of their radii) three forces act on particle $i$:

1. An elastic restoration force using a Hertzian contact law

\[
f_{el}^{(i)} = -Y\left(\frac{r_{ij}}{\sqrt{d_i + d_j}}\right)^{3/2},
\]

where $Y$ is the Young modulus and $r_{ij}$ points from particle $i$ to $j$;

2. A dissipation due to the inelasticity of the collision

\[
f_{diss}^{(i)} = -\gamma m_{eff} (v_{ij} \cdot r_{ij}) \frac{r_{ij}}{|r_{ij}|^2},
\]

where $\gamma$ is a phenomenological dissipation coefficient and $v_{ij} = v_i - v_j$ the relative velocity between the particles;

3. A shear friction force. In order to allow for static situations of blocking in a hopper due to arching it is important to include real static friction, i.e. which does not depend on the velocities but rather on the relative angle of the surfaces [32]. When two particles start to touch each other, one puts a “virtual” spring between the contact points of the two particles. Be $\delta s$ the total shear displacement of this spring during the contact and $k_s \delta s$ the restoring frictional force (static friction):

\[
f_{friction}^{(i)} = -k_s \delta s,
\]

where $\delta s$ is the shear displacement integrated over the entire collision time. The maximum possible value of the restoring force in the shear direction is then, according to Coulomb’s criterion, proportional to the normal force $F_n := f_{el}^{(i)} + f_{diss}^{(i)}$ multiplied by the friction coefficient $\mu$ [29,30]. Cast into a formula this gives a friction force

\[
f_{shear}^{(i)} = -\text{sign}(f_{friction}^{(i)}) \min(f_{friction}^{(i)}, \mu |F_n|).
\]

When particles are no longer in contact with each other the spring is removed. Since we found that omission of the rotational degree of freedom for our model does only slightly change the results quantitatively [24,25,28] we do not consider rotations here in order to save some computer time. In fact, when particles have strong deviations from the spherical shape rotations are strongly suppressed.

When a particle collides with a wall the same forces act as if it would have encountered another particle of diameter $d_0$ with infinite mass at the collision point. The inclined walls are in fact themselves made out of small particles and in order to introduce some wall roughness these particles are chosen randomly from a distribution of two radii $0.5$
and 1 mm, respectively, chosen each with probability 1/2. The only external force acting on the system is gravity $g \approx -10 \text{m/s}^2$.

We chose material parameters corresponding to aluminum spheres – stiffer solids would demand very small time steps and increase the need of computer time. So, we took a Young modulus of $Y = 10^8 \text{g/s}^2$ and a damping constant $\gamma = 500$, which corresponds to a restitution coefficient of 0.7. We set the friction parameters $\mu = 0.5$ and $k_s = 500, \ldots, 1000$ and use a time step of $\Delta t = 5 \times 10^{-6} \text{s}$. For all calculations we considered an output diameter of $D = 2 \text{cm}$ which is large enough to avoid clogging in most cases. Our program runs on various serial machines like SUN or IBM workstation clusters and on 8 or 16 processors of an Intel Paragon. We used a domain decomposition using strips for the parallelization and the efficiency became too low when more processors were used since the system sizes considered were too small [25].

As initial positions of the particles we considered them placed at random positions inside an area several times larger than needed for the dense packing. The initial velocities are set to zero. After that the particles are allowed to fall freely under gravity. Once they have settled to rest (after roughly 60,000 time steps which is equivalent to 0.3 seconds) we open the outlet at the bottom of the system and let the particles flow out. Each time the upper surface has moved down one layer this layer is refilled with particles at rest which gently fall down on the surface pulled by gravity. This refilling mechanism allows us to simulate rather long evolutions without noticeable deviations from steady state or unphysical side effects from periodic boundary conditions.

In Fig. 1 we see a snapshot of the granular medium flowing out of a hopper for two different angles for material parameters consistent with the experiment of Baxter et al. [12]. Shown are the contours of constant kinetic energy. We see the acceleration above the orifice and the formation of stagnation zones next to the walls. Interestingly, a short time after the opening of the outlet the stagnation zone is delimited by straight lines. Such a result was also observed with MD simulations without static friction (see Figs. 7 and 8 of Ref. [24]). The observed shapes of stagnation zones in real three
Fig. 2. Distributions of (a) pressures $p$ (normal forces) and (b) shear forces $\tau$ along the wall of the hopper, i.e. as function of the height $h$ in cm, at a given instant (0.165 s after opening the outlet) for $\theta = 40^\circ$. The upper curves correspond to the left wall and the lower curves to the right wall.

dimensional silos are however curved, either cusp-like downwards for primary flow or S-shaped for secondary flow [33]. After some time we see that indeed the shape of the stagnation zone becomes more S-shaped (Fig. 1a). Only close to the outlet the shape remains linear. The acceleration zones inside the flowing part have elliptic shape also in agreement with the observations of the inner core of the flow [33]. It seems that the fact that these observations were made on three dimensional hoppers while our numerical simulations are two dimensional (with exception of the Hertzian contact law) does not influence the qualitative picture very much.

It is interesting to see how the shape of the stagnation zone depends on the angle of the hopper $\theta$. For that sake we compare in Fig. 1 the case $\theta = 10^\circ$ and $\theta = 70^\circ$. In the case of a small angle the S-shape of the stagnation zone reaches down to the edge of the outlet. For large angles the wall gives a natural limitation to the slope of the stagnation zones as seen in Fig. 1b. This is the case of “mass flow” (no stagnation zones) as compared to “funnel flow” for which the material has to go through the funnel formed by the stagnation zones.

We measure the stresses acting against the walls by taking from our algorithm the normal ($p$) and tangential ($\tau$) components of the force acting against each of the particles of the walls and averaging these values over 1000 time steps. In Fig. 2 we see a typical snapshot of the distribution of these two components along the two walls as a function of height $h$. We see that both components have extremely strong variations. Along the upper part the stresses are in general weaker but the largest events occur at rather random locations and can attain forces of the order of 30 N. Unfortunately the hopper sizes we can numerically treat are not large enough to make a statistical analysis at a fixed time or to calculate the Fourier spectrum. We see from Fig. 2 that the normal components are between two and three times larger than the shear components.
in agreement with numerical work by Savage [34] in shear cells.

For practical purposes it is of more interest to monitor the time dependence of the stresses at a given position on the wall. In Fig. 3 we show the first invariant of the stress tensor, defined as $s := \sqrt{p^2 + \tau^2}$ as function of time measured at the height of the 10th wall particle above the edge of the outlet for $\Theta = 60^\circ$. The fluctuations are of the same order as the values themselves. No apparent correlations are visible. The distribution around the mean force is not Gaussian but an exponential. In order to get a more quantitative information we looked at the power spectrum of these time sequences, i.e. we took the square of the amplitude of its Fourier transformation. In Fig. 4 we see these spectra for two different angles. For sufficiently open hoppers, like for $\Theta = 40^\circ$, the spectrum decays with a power law $1/f^\alpha$ over at least one order of magnitude with an exponent that depends on $\Theta$ and the static friction coefficients $k_s$ and $\mu$. For $k_s = 500, \ldots, 1000$ and $\mu = 0.5$ the exponent $\alpha$ increases as 0.9, 1.5 and 1.8 for $\Theta = 60^\circ$, 40° and 10°, respectively. This is consistent with the experimental results of Baxter et al. [12] who worked at an opening angle of 45° ($\Theta = 67.5^\circ$) and found an exponent in the range of $\alpha = 1.3, \ldots, 2.3$ for different situations. Their power laws, however, extend over a much larger range than in our case because the computer requirements limited our observation times to several seconds while the real experiments can be carried out over many hours.

It is very interesting to note that if the hopper walls become more inclined (Fig. 4b) the spectrum changes abruptly and becomes white noise. Savage [34] found a similar situation in numerical calculations of the wall stresses in shear cells as function of density: Only at rather high densities the power spectrum showed a power law while for lower densities he observed white noise. In our case, although the density cannot be varied, a change in the opening angle determines if there are stagnation zones or not and evidently the density in the flowing regions is lower than in stagnations zones. Also
higher up along the walls where the stagnation zones become thicker the validity of the power law behaviour, i.e. the range in frequencies, increases.

Investigating with large scale MD simulations the force distribution and the shape of the stagnation zones of outflowing hoppers we have found an interesting dependence on the opening angle: In the case of funnel flow (e.g. $\Theta = 75^\circ$) there are no stagnation zones and the power spectrum of the stresses against the walls has white noise. Opening the angle one finds stagnation zones and a power law spectrum. In addition the range of the power law behaviour increases for increasing height. This leads one to suspect that the power law in the stress spectrum does not originate from the power law in the density fluctuations [4,31] because the density fluctuations also follow a power spectrum in the case of funnel flow. It seems more likely that the stagnation zones act like “noise transformers” in which essentially uncorrelated random kicks coming from the outflowing core are transmitted through the complex contact network to the wall and arrive power-law correlated. Similar observations have been made with the propagation of shock and sound waves in dense packed boxes [11].

The shape of the stagnation zones agree qualitatively very well with experimental observations. Although our simulations are two dimensional, it seems that our model does capture the essential mechanisms that occur in three dimensional experiments.

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