Langevin equation approach to granular flows in narrow pipes

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The flow of granular material through a rough narrow pipe is described by the Langevin equation formalism. The stochastic force is caused by irregular interaction between the wall and the granular particles. In correspondence with experimental observations we find clogging and density waves in the flowing material.

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When granular material flows through a narrow vertical pipe one observes recurrent clogging and density waves. This effect is well known to physicists and engineers, usually it is undesirable and causes technological problems, e.g. in chemical engineering. Density waves play a major role in the behavior of granular materials and have been investigated by many authors using various methods:

Ristow and Herrmann reproduced the density fluctuations in an out-flowing hopper by molecular dynamics that have been observed experimentally before (e.g.) using the X-ray technique. Baxter and Behringer simulated the flow using an cellular automaton. Peng and Herrmann studied a Lattice Gas Automaton for the flow of granular material. Using phenomenologically plausible rules for the interaction of particles and of particles with the wall they could reproduce density fluctuations which spectrum obeys a power law. Lee and Leibig applied the kinetic wave approach to the flow of granular particles through a pipe. They treated initial random density fluctuations as a set of distinct homogeneous density regions and considered the motion of the interfaces between them. Finally they could show, that the evolution of such a simple model leads to the formation of clusters with a high density contrast.

The aim of the present paper is to provide a model for the flow of granular material in a vertical narrow pipe using the Langevin-equation approach of stochastic forces. Such a approach was also used by Mehta et al. to describe the relaxational behavior of a granular pile submitted to vibration and was proved to be suitable. We will show that our model is able to reproduce the experimental observations. The simulation of the resulting density equation requires much less computational effort than the direct simulation using molecular dynamics. We discuss the instability of the homogeneous flow in the hydrodynamic approximation and provide critical values for the occurrence of clogging and density waves.

When sand flows through a narrow pipe we assume that there is a permanent random interaction of the sand particles with the wall of the pipe. The equations of motion for a single particle which is subjected to gravity $g$ in positive $x$-direction and which does not interact with other particles in the low density regime read

\[ \dot{x}_i = v_i \]
\[ m \dot{v}_i = mg - \gamma v_i + \sqrt{2 \gamma} \xi_i(t). \]

The friction $\gamma$ and the Langevin fluctuation term results from the interaction of the grain with the wall. (Although our model does not include the interaction of the grains with the air inside the pipe, in a very simple approximation one can assume that the fluctuation term accounts for this interaction too.) For the stochastic force we assume Gaussian white noise $\langle \xi_i(t) \xi_j(t+T) \rangle = \delta_{ij} \delta(T)$. The path of a particle is scattered independently at different places during its motion downwards which is described by independent impacts in time. Hence, after the relaxation time $m/\gamma$ the velocities of the particles obey a Maxwellian distribution with mean value $v^0 = mg/\gamma$.

We apply the collision integral proposed by Prigogine and Herman for the description of particle interactions. In their investigation it was intended to model vehicular traffic flow and it has been pointed out by several authors (e.g.) that traffic flow on one-lane highways reveals striking similarities to granular flow in a pipe. When a fast moving particle $i$ collides with a slower one $j$ after the collision both grains move with the lower velocity $v_j$.

\[ \bigcirc v_i \rightarrow \bigcirc v_j \Rightarrow \bigcirc \bigcirc v_j \]

During the impact the momentum balance of the particles is not conserved. Due to the strong interaction between the particle and the wall we suppose that the lost part of the momentum will be taken over by the wall which is assumed to be coupled with a reservoir. Introducing the effective cross section $C$ which depends on the geometry of the pipe and the particles the collision integral reads

\[ \frac{\partial P}{\partial t} \sim \int_{-\infty}^{\infty} P(x,v,t) P(x,v',t) (v' - v) \, dv' \]
\[ = C \, P(x,v,t) n(x,t) (u(x,t) - v), \]
where \( P(x,v,t) \) is the one-particle probability density in phase space. The particle density \( n(x,t) \) and the mean velocity \( u(x,t) \) at position \( x \) and time \( t \) are given by

\[
\begin{align*}
n(x,t) &= \int_{-\infty}^{\infty} P(x,v,t) \, dv \\
u(x,t) &= \frac{1}{n(x,t)} \int_{-\infty}^{\infty} v \, P(x,v,t) \, dv.
\end{align*}
\] (3a, 3b)

Hence we find the kinetic equation

\[
\frac{\partial P}{\partial t} + \frac{\partial}{\partial x}[vP] + \frac{\partial}{\partial v} \left[ (g - \frac{\gamma}{m} v) P \right] = \frac{\epsilon \gamma}{m^2} \frac{\partial^2 P}{\partial v^2} + CP(x,v,t)n(x,t)(u(x,t) - v)
\] (4)

and in a homogeneous stationary flow \((n = n^0, u = u^0)\)

\[
P^0(v) = \sqrt{\frac{m}{2\pi k_B T^0}} \exp\left( -\frac{m}{2 k_B T}(v - u^0)^2 \right). \tag{5}
\]

The mean velocity

\[
u^0 = \frac{mg}{\gamma} - \frac{C k_B T^0 n^0}{\gamma} \tag{6}
\]

depends on the density and the mean square displacement of the velocity:

\[
T(x,t) = \frac{m}{k_B n(x,t)} \int_{-\infty}^{\infty} (v - u(x,t))^2 P(x,v,t) \, dv. \tag{7}
\]

In the homogeneous case we find

\[
T = T^0 = \frac{\epsilon}{k_B}. \tag{8}
\]

Therefore the homogeneous flux through the pipe

\[
j^0 = n^0 u^0 = n^0 \left( \frac{mg}{\gamma} - \frac{C k_B T^0}{\gamma} n^0 \right) \tag{9}
\]

shows two distinct regimes: a low density regime due to a high particle velocity where only very few collisions occur and a high density regime due to low particle velocity caused by dissipative impacts of particles.

When we assume local equilibrium, i.e. \( n^0 \to n(x,t), u^0 \to u(x,t) \), and \( T^0 \to T(x,t) \), we rewrite eq. (4):

\[
\frac{\partial P}{\partial t} + \frac{\partial}{\partial x}[vP] + \frac{\partial}{\partial v} \left[ \left( \frac{F(n,T)}{m} - \frac{\gamma}{m} v \right) P \right] = \frac{\epsilon \gamma}{m^2} \frac{\partial^2 P}{\partial v^2}.
\] (10)

Similar as in the Vlassov formulation \([4]\) the force

\[
F(n,T) = mg - C k_B T(x,t)n(x,t) \tag{11}
\]

is determined to be self-consistent in its dependence on density and granular temperature of the material. With the effective force \( F(n,T) \) acting on the particles at a given location \( x \) and a given time \( t \) we find the corresponding Langevin equation for the motion of the particles which are subjected to gravity and impacts of other grains

\[
\dot{x}_i = v_i
\]

\[
m \dot{v}_i = -\gamma v_i + F(n(x_i,t), T(x_i,t)) + \sqrt{2\epsilon \gamma} \xi_i(t).
\] (12)

Eqs. (11,12) determine an effective simulation algorithm (for details see \([5]\)).

From eq. (10) we derive the hydrodynamic equations

\[
\begin{align*}
\frac{\partial n}{\partial t} + \frac{\partial}{\partial x}[nu] &= 0, \\
\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} &= \frac{F(n,T)}{m} - \frac{\gamma}{m} \frac{\partial}{\partial x}[nT],
\end{align*}
\] (13a, 13b)

\[
\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} = \frac{2\gamma}{m} \frac{\partial u}{\partial x} - 2\epsilon \frac{\partial}{\partial x} \frac{\partial}{\partial x} + \frac{\partial}{\partial x} \epsilon \frac{\partial^2 n}{\gamma \partial x^2}. \tag{13c}
\]

The first two terms on the right hand side of the heat balance equation (13c) describe the heat exchange between the granular material and the wall, whereas the last term leads to an effective volume viscosity.

In the approximation of quick temperature and velocity relaxation one finds for the high damping limit \((\gamma \to \infty)\) the Burgers equation

\[
\frac{\partial n}{\partial t} + \frac{1}{\gamma} \frac{\partial}{\partial x} F(n,T) = \frac{\epsilon}{\gamma} \frac{\partial^2 n}{\partial x^2}. \tag{14}
\]

In this limit there are no self sustained inhomogeneous solutions of eq. (13) (see \([4]\)). For finite damping, \(\gamma < \infty\), however, as shown below the homogeneous solution \( n = n^0, u = u^0, T = T^0 \) of the eqs. (13) becomes unstable when the average density approaches a critical value \( n^{cr} \). In the context of clustering instabilities in dissipative gases Goldhirsch and Zanetti \([7]\) argued similarly: when the pressure in a dense region decreases due to dissipation, the resulting pressure gradient leads to further increase of the density which finally results in a granular cluster.

In the following we want to discuss the stability analysis of the hydrodynamic equations (13) \([8,9]\). Obviously, there is a homogeneous solution \((n^0, u^0, T^0)\) for a given homogeneous density \( n^0 \). We disturb the homogeneous state in eqs. (13) with wave-like perturbations \((\delta n \sim \delta u \sim \delta T \sim \exp(-\alpha t + ikx))\), drop the quadratic terms and get an eigenvalue–problem for \(\alpha(k)\). If the real part of \(\alpha(k)\) is negative, \(\text{Re}(\alpha(k)) < 0\), fluctuations can grow and the initially homogeneous state becomes unstable. The transition occurs at the critical particle density \( n^{cr} \) where \(\text{Re}(\alpha(k)) = 0 \). Because of the assumed periodic boundary conditions the wavenumber \( k \) is discrete: \( k = \frac{2\pi i}{L} \quad (i = \pm 1, \pm 2, \ldots) \). Fig. 1 shows the critical density \( n^{cr} \) over the dimensionless mode number \( i \). Obviously in particular short length perturbations are able to destabilize the homogeneous flow in the granular system.
This stands in strong contrast to results found for hydrodynamic formulations for traffic [13,19,20] and granular flows [22], where the long range fluctuations are the critical ones. Our results are not surprising if one imagines that a local large gradient of the velocities will lead to a high collision rate at this place. For sufficient high density this process leads to clusters with high local density and small average velocity.

For large wave numbers we get a low limiting critical density given by

$$\lim_{|k| \to \infty} n^c_r(k) = \frac{7}{3\sqrt{3}} \frac{\gamma}{\sqrt{\epsilon mC}} = \frac{7}{3\sqrt{3}} L_B C,$$  \hspace{0.5cm} (15)

where $L_B = \sqrt{\epsilon \frac{m}{\gamma}}$ is the braking distance, i.e. the length a particle is damped out after an impact. It determines the length scale which characterizes our granular system and its critical behavior. In contrast, the critical behavior of the traffic flow models proposed in [13,19,20] depends on the length $L$ of the entire (periodic) system too since the critical fluctuations are long range ones.

To check the analytic results the time–discretized Langevin equations

$$x_i(t + \Delta t) = x_i(t) + v_i(t)\Delta t  \hspace{0.5cm} \text{(16a)}$$

$$v_i(t + \Delta t) = v_i(t) + \left(\frac{F(n,T)}{m} - \frac{\gamma v_i(t)}{m}\right)\Delta t +$$

$$\frac{\sqrt{2\gamma \Delta t}}{m}\text{GRND} \hspace{0.5cm} \text{(16b)}$$

have been solved numerically. GRND is a Gaussian random number with standard deviation equal unity. Using the parameters $m = 7.4 \times 10^{-7} \text{ kg}$, $\gamma = 7 \times 10^{-6} \text{ kg/sec}$, $\epsilon = 2.0 \times 10^{-8} \text{ Nm}$, $C = 6.4 \times 10^{-3}$, $g = 9.81 \text{ m/sec}^2$, and $\Delta t = 0.01 \text{ sec}$ we calculated the time dependent density, velocity and granular temperature from the trajectories of the Brownian particles. The given parameters have been determined experimentally [18]. We assume periodic boundary conditions and homogeneous initial conditions. Inserting the given parameters into eq. (17) we find $n^c_r = 12000/m$.

Fig. 2 shows the velocity distributions

$$w(v,t) = \int_0^L P(x,v,t)dx$$  \hspace{0.5cm} (17)

of a stable (undercritical) ($n^0 = 11000/m < n^c_r$) and an unstable system ($n^0 = 14000/m > n^c_r$). In the undercritical case we find a stable homogeneous flow with Gaussian velocity distribution, while in the latter case inhomogeneities due to random fluctuations increase with time and the velocity distribution $w(v,t)$ is no longer Gaussian. In our opinion there are at least two distinct velocity distributions in the system: at regions of low density we find high average grain velocity and at high density regions the grains move with low average velocity. The overlayed curves in the distribution plots (fig. 3)

show support of the assumption of a bimodal velocity distribution.

Fig. 3 shows snapshots of the particle density of the unstable system where gravity acts in positive $x$-direction. We eventually observe the formation of two moving clusters originating from random inhomogeneities in the early state of the system–evolution. In dependence from the initial conditions we found also configurations with one or three moving clusters. In correspondence with the experiment and MD simulations [2] we observed coexisting clusters moving either in positive or negative direction. Note that the slope at the left hand side of the density wave in fig. 3 is very steep. Here the collision rate is very high due to the large velocity gradient between the particles which are involved in the clusters and the free falling ones (fig. 1). The particle velocity at the right hand side of the clusters is much lower. There the grains’ velocity slowly increases under the influence of gravity and hence the high density area, i.e. the cluster, dissolves (see also [23]). These processes lead to the obvious hump-like shape of the clusters in fig. 6. Contrary to the hump-like solutions of the Burgers-equation [16] the widths of the clusters remains invariant when they move through the pipe. Fig. 3 shows the described sharp decrease and slowly increase of the particle velocities. As one can derive from the hydrodynamic equations (13c) the high negative velocity gradient at the front (left hand side) of a cluster leads to an increase of the granular temperature, whereas the small positive velocity gradient inside and at the backside of the cluster results in a smaller granular temperature compared with outside the clog. Fig. 4 (lower part) illustrates this plausible behavior.

We investigated the granular flow through a vertical narrow pipe using a simple model consisting of Brownian particles with collision interaction. We could show that there is a critical value for the particle density which decides whether a initially homogeneous flow remains stable. The model is valid in the limit of pairwise particle interaction. This precondition is assumed to be fulfilled for the case of moderate particle density and low pipe width. Our model also defines an efficient simulation method for granular flows. Applying this algorithm to low- and high-density pipe flow we found that in both cases the numerical results agree with the theoretical prediction. The numerical results for the spacial particle density, the average velocity, and the granular temperature agree with the hydrodynamic description.

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FIG. 1. The critical density $n_{cr}$ over the mode number $i$. The parameters are $m = 7.4 \times 10^{-7}$ kg, $\gamma = 7 \times 10^{-6}$ kg/sec, $\epsilon = 2.0 \times 10^{-8}$ Nm, $C = 6.4 \times 10^{-3}$, $g = 9.81$ m/sec$^2$. For different parameters the curve changes, however, its qualitative shape remains conserved.

FIG. 2. Velocity distribution found by simulations of the stable homogeneous and the unstable system (solid lines) and the corresponding analytical results (dashed lines).

FIG. 3. The particle density of the unstable system at times $t = 4$ sec and $t = 500$ sec. Since the initial (homogeneous) density is overcritical the inhomogeneities increase with time.

FIG. 4. The mean velocities (top) and the mean square displacement of the velocity (bottom) of the unstable system at time $t = 500$ sec.