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Langevin Equation Approach to Granular Flow in a Narrow Pipe

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The gravity-driven flow of granular material through a rough, narrow vertical pipe is described using the Langevin equation formalism. Above a critical particle density the homogeneous flow becomes unstable with respect to short-wave length perturbations. In correspondence with experimental observations, we find clogging and density waves in the flowing material.

KEY WORDS: Granular material; stochastic processes; flow of solids.

Granular materials show complex and sometimes unexpected behavior in many situations and therefore have attracted much scientific interest (e.g., refs. 1–3). When granular material flows through a narrow vertical pipe one observes recurrent clogging and density waves.[4-6] 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: Using molecular dynamics, Ristow and Herrmann[7] reproduced density fluctuations in an outflowing hopper which had been previously observed experimentally (e.g., ref. 8). Baxter and Behringer[9] simulated the flow with cellular automata. Peng and Herrmann[10] studied a lattice gas automaton[11] for the flow of granular material. Using phenomenologically plausible rules for the interaction of particles and of particles with the wall, they reproduced density fluctuations whose spectrum obeys a power law. Lee and Leibig[12] applied the kinetic wave approach[13] to the flow of granular particles through a

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pipe. They treated initial random density fluctuations as a set of distinct homogeneous density regions and considered the motion of the interfaces between them. They showed that the evolution of such a simple model leads to the formation of clusters with high-density contrast.

The aim of the present paper is to provide a one-dimensional model for the gravity-driven flow of granular material in a vertical narrow pipe using the Langevin-equation approach of stochastic forces. Such an approach was successfully used by Mehta *et al.*[14] to describe the relaxation of a granular pile subjected to vibration. In our description we do not consider the interaction of the sand with another medium such as air. Although it has been stated that air has major influence on the clogging behavior (e.g., ref. 6), we will show that our model is able to reproduce qualitatively the experimental observations.[4,5] To our knowledge there are no experimental data which describe the flow of sand in an evacuated pipe. Starting from the Langevin formalism, we derive an expression for the grain density. 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 subjected to gravity g in the positive x direction which does not interact with other particles in the low-density regime read

$$\dot{x}_i = v_i \tag{1a}$$

$$m\dot{v}_i = mg - \gamma v_i + \sqrt{2\varepsilon\gamma}\,\xi_i(t) \tag{1b}$$

The friction γ and the Langevin fluctuation term are effective forces resulting from the interaction of the single grain with the wall. For the stochastic force we assume Gaussian white noise $[\langle \xi_i(t)\,\xi_j(t+T)\rangle = \delta_{ij}\,\delta(T)]$. We assume that during its motion through the pipe the particle impacts the wall independently at different places. This behavior is described as independent impacts in time. Hence, after relaxation time m/γ the velocity of the particle obeys a Maxwellian distribution with mean $v^0 = mg/\gamma$.

Besides the interaction of the grains with the wall, the particle–particle interaction has to be considered. Here we apply the collision integral proposed by Prigogine and Hermann.[15][2] After a collision the faster particle i adopts the velocity of the slower one j,

$$\bigcirc \xrightarrow{v_i} \bigcirc \xrightarrow{v_j} \Rightarrow \bigcirc\bigcirc \xrightarrow{v_j}$$

[2] Here the collision integral was intended to model vehicular traffic. It has been pointed out by several authors (e.g., refs. 26 and 5) that traffic flow on one-lane highways reveals striking similarities to granular flow in a pipe.

The proposed mechanism does not conserve momentum. Since the pipe explicitly does not belong to the system described by Eqs. (1) we assume that momentum is balanced via inelastic collisions with the wall.

With the mean values for the particle velocity $u(x, t)$, density $n(x, t)$, and granular temperature $T(x, t)$ at position x at time t

$$n(x, t) = \int_{-\infty}^{\infty} P(x, v, t)\, dv \tag{2a}$$

$$u(x, t) = \frac{1}{n(x, t)} \int_{-\infty}^{\infty} vP(x, v, t)\, dv \tag{2b}$$

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

we write the Boltzmann equation for the one-particle probability density $P(x, v, t)$

$$\begin{aligned} \frac{\partial P}{\partial t} + \frac{\partial}{\partial x}(vP) + \frac{\partial}{\partial v}\left[\left(g - \frac{\gamma}{m} v\right) P\right] - \frac{\varepsilon\gamma}{m^2} \frac{\partial^2 P}{\partial v^2} &= C \int_{-\infty}^{\infty} P(x, v, t)\, P(x, v', t)(v' - v)\, dv' \\ &= CPn(u - v) \end{aligned} \tag{3}$$

The effective cross section C is a complex function of the pipe geometry and the properties of the particles which has to be determined experimentally. Since we do not investigate the influence of the properties of the pipe and the grain material on the flow characteristics, we may treat this value as a constant.

Equation (3) has the stationary solution

$$P^0(v) = \left(\frac{m}{2\pi k_B T^0}\right)^{1/2} n^0 \exp\left[-\frac{m}{2k_B T^0}(v - u^0)^2\right] \tag{4a}$$

$$u^0 = (mg - Ck_B T^0 n^0)\, \gamma^{-1} \tag{4b}$$

$$T^0 = \varepsilon k_B^{-1} \tag{4c}$$

The homogeneous flux through the pipe

$$j^0 = n^0 u^0 = n^0 \left(\frac{mg}{\gamma} - \frac{Ck_B T^0}{\gamma} n^0\right) \tag{5}$$

therefore reveals two regimes: a low-density regime with high particle velocity where only very few collisions occur, and a high-density regime with low particle velocity caused by dissipative impacts of particles.

With the assumption of local equilibrium we insert the solution (4a) in (3),

$$\frac{\partial P}{\partial t}+\frac{\partial}{\partial x}(vP)+\frac{\partial}{\partial v}\left[\left(\frac{F(n,T)}{m}-\frac{\gamma}{m}v\right)P\right]-\frac{\varepsilon\gamma}{m^2}\frac{\partial^2 P}{\partial v^2}=0 \tag{6}$$

The acceleration due to gravity has to be replaced by the self consistent local force $F(n, T)$ acting on the particles at a given location x and a given time t,

$$F(n,T)=mg-Ck_B T(x,t)\,n(x,t) \tag{7}$$

Inserting in (1a), we find the Langevin equation for the motion of particles which are subjected to gravity and impacts of other grains

$$\dot{x}_i=v_i \tag{8a}$$

$$m\dot{v}_i=-\gamma v_i+F(n(x_i,t),T(x_i,t))+\sqrt{2\varepsilon\gamma}\,\xi_i(t) \tag{8b}$$

in correspondence with Eq. (6). Hence, Eqs. (8) describe the motion of a single particle affected by the fields $n(x, t)$ and $T(x, t)$.

We derive the hydrodynamic equations from Eq. (6):

$$\frac{\partial n}{\partial t}+\frac{\partial}{\partial x}(nu)=0 \tag{9a}$$

$$\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}=\frac{F(n,T)}{m}-\frac{\gamma}{m}u-\frac{k_B}{mn}\frac{\partial}{\partial x}(nT) \tag{9b}$$

$$\frac{\partial T}{\partial t}+u\frac{\partial T}{\partial x}=-\frac{2\gamma}{m}T+\frac{2\varepsilon\gamma}{mk_B}-2T\frac{\partial u}{\partial x} \tag{9c}$$

The first two terms on the rhs of the heat balance equation (9c) describe the heat exchange between the granular material and the wall, whereas the last term leads to an effective volume viscosity. We recall that our model is one dimensional, hence the viscosity is an effective value which accounts for the energy loss due to impact of particles. In the approximation of rapid temperature and velocity relaxation for the high-damping limit ($\gamma \to \infty$), Eqs. (9) reduce to the Burgers equation

$$\frac{\partial n}{\partial t}+\frac{1}{\gamma}\frac{\partial}{\partial x}F(n,T^0)=\frac{\varepsilon}{\gamma}\frac{\partial^2 n}{\partial x^2} \tag{10}$$

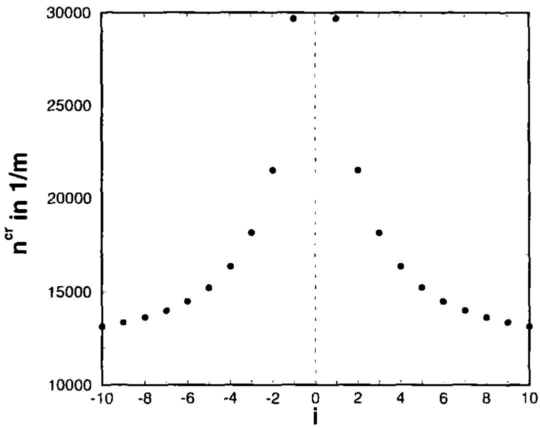

Fig. 1. The critical density n^{cr} over the mode number i of a perturbation. The homogeneous solution is sensitive in particular with respect to short-length perturbations. The parameters are $m = 7.4 \times 10^{-7}$ kg, $\gamma = 7 \times 10^{-6}$ kg/sec, $\varepsilon = 2 \times 10^{-8}$ N m, $C = 6.4 \times 10^{-3}$, and $g = 9.81$ m/sec^2. For different parameters the curve changes; however, its qualitative shape remains conserved.

In this limit (10) does not have self-sustained inhomogeneous solutions.[16] For finite damping, however, as shown below, the homogeneous solution n^0, u^0, T^0 of Eqs. (9) becomes unstable when the average density approaches a critical value n^{cr}.[17]3

We have shown that there is a homogeneous solution (4a) for a given homogeneous density n^0. Now we want to discuss the stability[18] of the hydrodynamic equations (9) with respect to a wavelike perturbation

$$\delta n \sim \delta u \sim \delta T \sim \exp(-\alpha t + ikx), \qquad k = 2\pi i/L \quad (i = \pm 1, \pm 2, ...) \quad (11)$$

in linear approximation, which leads to an eigenvalue problem for $\alpha(k)$. (Because of the assumed periodic boundary conditions the wavenumber k is discrete.) For density $n > n^{cr}$ fluctuations can grow and the homogeneous state is unstable, $\mathrm{Re}[\alpha(k)] < 0$. Figure 1 shows the critical density over the mode number i. Obviously in particular short-length perturbations destabilize the homogeneous flow. This stands in strong contrast to results found for hydrodynamic formulations of vehicular traffic[15, 19, 20] and granular flows,[21] where the long-range fluctuations are the critical ones. Our results are not surprising if one imagines that a local large gradient of

3 In the context of clustering instabilities in dissipative gases the authors 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.

the velocities will lead to a high collision rate at this place. For sufficiently 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

$$\lim_{|k| \to \infty} n^{cr}(k) = \frac{7}{3\sqrt{3}} \frac{\gamma}{\sqrt{\varepsilon m}\, C} = \frac{7}{3\sqrt{3}} \frac{1}{L_B C} \tag{12}$$

where $L_B = \sqrt{\varepsilon m}/\gamma$ is the relaxation length, i.e., the distance after which the information of an impact the particle has undergone is damped out. It can be considered to be the length scale which characterizes our granular system and its critical behavior. In contrast, the critical behavior of the traffic flow models proposed in refs. 15, 19, and 20 depends on the length L of the entire (periodic) system, too, since the critical fluctuations in these systems are long-range ones.

To check the analytic results, the discretized Langevin equations

$$x_i(t + \Delta t) = x_i(t) + v_i(t)\, \Delta t \tag{13a}$$

$$v_i(t + \Delta t) = v_i(t) + \left(\frac{F(n(x_i, t), T(x_i, t))}{m} - \frac{\gamma v_i(t)}{m} \right) \Delta t + \frac{(2\varepsilon\gamma\, \Delta t)^{1/2}}{m}\, \mathrm{GRND} \tag{13b}$$

have been solved numerically (for a detailed description of the algorithm see ref. 22). GRND is a Gaussian random number with standard deviation equal to unity. For the parameters $m = 7.4 \times 10^{-7}$ kg, $\gamma = 7 \times 10^{-6}$ kg/sec, $\varepsilon = 2 \times 10^{-8}$ Nm, $C = 6.4 \times 10^{-3}$, $g = 9.81$ m/sec^2, and $\Delta t = 10^{-2}$ sec we find by means of (12) $n^{cr} = 12{,}000/m$. The given parameters have been determined experimentally.[18] During the simulation the density and the temperature were found by coarse graining in small boxes due to Eqs. (2). The box width is small with respect to the relaxation length L_B.

Figure 2 shows the velocity distributions

$$w(v, t) = \int_0^L P(x, v, t)\, dx \tag{14}$$

of a stable (undercritical) and an unstable system. 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

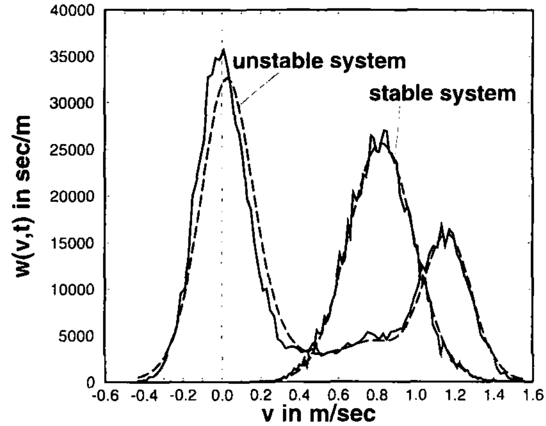

Fig. 2. Velocity distribution found by simulations of a stable homogeneous system ($n^0 = 11{,}000/m < n^{cr}$) and an unstable system ($n^0 = 14{,}000/m > n^{cr}$) (solid lines). The dashed line shows the (normalized) sum of two Maxwellian distributions due to Eq. (4a) whose characteristics n, u, and T have been extracted from simulations.

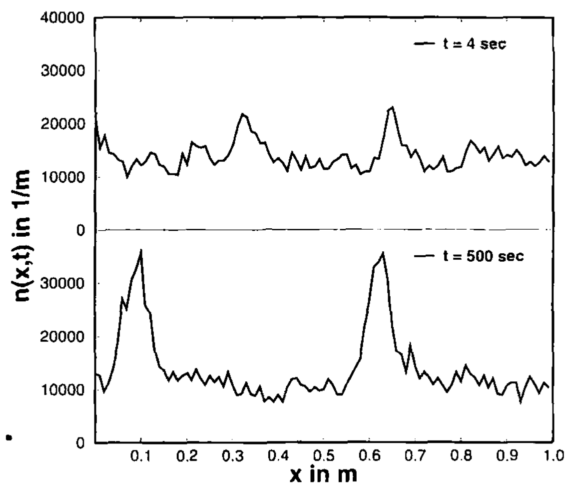

Fig. 3. The particle density of the unstable system at times $t = 4$ and 500 sec. Since the initial (homogeneous) density is overcritical, the inhomogeneities increase with time and eventually form stable clusters. The clusters can move up- or downwards and their number changes by fusion or separation. These processes are strictly stochastic, hence they cannot be described within the hydrodynamic approximation [Eqs. (9)].

velocity. Both regimes are sharply separated from each other and can be assigned separate sets of averaged density (n_l^0, n_h^0), velocity (u_l^0, v_h^0), and granular temperature (T_l^0, T_h^0), respectively. The dashed line in Fig. 2 shows the normalized superposition of two Gaussian distributions where the parameters n, u, and T come from simulations in the high-and low-density regimes.

Figure 3 shows snapshots of the particle density of the unstable system. Starting at time $t = 0$ with a homogeneous distribution, after some time we eventually observe the formation of two moving clusters originating from random inhomogeneities. Depending on the initial conditions, we find configurations with one or three moving clusters, too. In correspondence with experiments[18, 5] and MD simulations,[5] we observed coexisting clusters moving either in positive or negative direction.

Figure 4 shows snapshots of the particle velocities and granular temperatures which correspond to the lower part of Fig. 3. Note that the slope of both curves at the left-hand side of the density wave 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. The particle velocity at the right-hand side of the clusters is much lower. There the grain velocity slowly increases under the influence of gravity and hence the high density area, i.e., the cluster, dissolves (see also ref. 23). These processes lead to the hump shape of the clusters in Fig. 3. Contrary to the humplike solutions of the Burgers equation,[16] the widths of the clusters

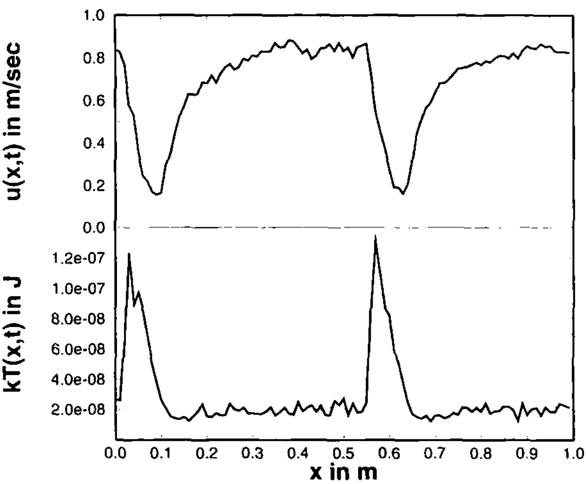

Fig. 4. Snapshot of the velocity (top) and the mean square displacement of the velocity (granular temperature) (bottom) of the unstable system at time $t = 500$ sec.

remain invariant when they move through the pipe. The high negative velocity gradients at the front (left-hand side) of a cluster lead to an increase of the granular temperature (Fig. 4), whereas the small positive velocity gradient inside and at the back of the cluster results in a smaller granular temperature as compared with outside the clog.

The simulation of the time-discretized Langevin equations (13) does not require time-consuming evaluation of forces as in the case of the full molecular dynamics (e.g., refs. 24 and 25). When numerically solving Eqs. (13) the only time-consuming part of the algorithm is the calculation of density, velocity, and temperature fields from the positions and velocities of the Brownian particles by coarse graining. For the calculation presented here we measured a speedup factor of about 80–90 of the presented method as compared with MD.

We investigated the gravity-driven granular flow through a vertical narrow pipe using a simple model consisting of Brownian particles with collision interaction. We showed that there is a critical value for the particle density which decides whether 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. Simulations of the discretized Langevin equation for low and high density support the theoretical prediction. The numerical results for the spatial particle density, the average velocity, and the granular temperature agree with the hydrodynamic description. 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 in the Langevin equation accounts for this interaction, too.

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