Stochastic analysis of single particle segregational dynamics

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Received 13 December 2004; accepted 5 January 2005
Available online 18 January 2005
Communicated by J. Flouquet

Abstract
Inverse grading in hard sphere granular flow is described by an effective stochastic process for the vertical displacement of particles in time. By pure, parameter-free data analysis, we extract an underlying stochastic Langevin equation for the heights dynamics of large and small particles. Fixed points of the deterministic vertical dynamics of individual particles are determined and show that within this macroscopic description of a granular flow, inverse grading of large particles is due to a deterministic effect. These results may be used as an efficient alternative to time consuming direct numerical modelling of inverse grading.

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1. Introduction

One of the most prominent and counter-intuitive features of flowing granular material is the effect of inverse segregation [1]. That is, granular materials moving under the influence of gravity tend to segregate in such a way that larger particles are more likely to be found at the top of the flow, whereas the smaller ones preferably accumulate near the bottom. The effect of inverse grading is of importance in industrial mixing and separation processes [2,3] as well as in a geological context, for example in rockfalls [4–6] or in snow flow avalanches [7–9].

In this contribution, we use a numerical simulation based on a simple hard sphere model of rapid granular flow. Despite its simplicity, the numerical model is able to reproduce the effect of inverse grading. Here we prove this by considering the time evolution of the mean particle radius profiles of the moving model flow and furthermore by a detailed stochastic analysis of the time dynamics of individual particles of different sizes. In particular, we show that from the given time series, the effective stochastic process can be reconstructed in a parameter-free way.

This Letter is structured as follows: first the numerical model is presented, second the method of the...
used stochastic analysis is presented and subsequently applied to the analysis of the motion of two typical segregating particles.

2. Numerical model of the granular flow

In the following, we confine ourselves to rapid granular flows in the “inertial regime” [10] which are mainly governed by binary particle collisions. This means that the flow can be simulated by tracing the ballistic trajectories of all freely moving particles in the flow until one particle collides with another. The collision is assumed to happen at a singular point in time. In the frame of this approach, the dynamics (i.e., the transverse and angular momenta) of two colliding particles after a binary collision are computed using the conservation of momentum with respect to the inelastic material properties of the particles. This method is termed “hard sphere modelling” and is well suited to the modelling of rapid granular flows in the inertial regime [11–13]. The binary collisional interactions between the particles are parametrised using the particle material parameters \( e, b, \mu \), where \( e \) and \( b \) denote the longitudinal and tangential coefficients of restitution of a particle and \( \mu \) is the Coulomb coefficient of tangential friction between surfaces of colliding particles. A laterally infinite flow was modelled by tracing 212 particles with a continuous radius distribution in the range \( r_i \in [0.18, 0.3] \) in an inclined box with periodic boundary conditions and periodicity lengths \( l_x = 4 \) and \( l_y = 2 \). The \( z \)-coordinate, which henceforth is also referred to as “vertical direction”, is perpendicular to the inclined bottom of the box and will be labelled by \( h \). The box is inclined by an angle \( \psi = 28^\circ \) and its bottom is roughened by attaching semi-spheres with a diameter of 0.4 to it. (Length units have been skipped and all lengths are understood to be in units of m.) The particle size distribution used in the simulations is shown in Fig. 1(a).

With the material parameters \( e, b, \mu \) of the particles set to \( e = 0.8, b = 0.7, \mu = 0.4 \), a steady flow with a mean downslope velocity \( v_x \approx 7 \text{ ms}^{-1} \) was achieved after a model running time of \( t = 40 \text{ s} \). The total running time of the simulation was 980 s. For details and for a parameter space study of the model refer to [8,14]. The inverse grading taking place in this model flow is reflected by the time evolution of the \( h \)-dependence of the mean particle radius, \( \langle r(h) \rangle \), as shown in Fig. 1(b).

3. Stochastic analysis

Next, the height dynamics, \( h(t) \), of the trajectories of individual particles are considered. In particular, we focus on a large and a small particle, whose vertical trajectories are shown in Figs. 2(a) and 3(a). To grasp the content of these apparently random trajectories, we make use of a stochastic analysis introduced recently for the analysis of turbulence and noisy chaotic dynamics [15–18]. Basic introduction to stochastic processes is provided by [19–21].

![Fig. 1](image-url)
Fig. 2. Analysis of large particle dynamics: (a) normalised time series of particle elevation $h^* = h/h_{\text{max}}$, (b) probability of elevation $p(h^*)$, (c) drift term $D^{(1)}(h^*)$, (d) effective potential $V(h^*)$, (e) diffusion term $\sqrt{D^{(2)}(h^*)}$. Stable fixed points at elevations $h^* = 0.37$ and $h^* = 0.53$ are marked by arrows.

Fig. 3. Same as in Fig. 2 but for a small particle.

For this approach, it has to be shown that the underlying dynamics of single particles have Markovian properties, i.e., for a time sequence $t_1 < t_2 < \cdots < t_n$ with corresponding height values $h_1, \ldots, h_n$ of an individual particle the relation

$$p(h_n, t_n | h_{n-1}, t_{n-1}; \ldots; h_1, t_1) = p(h_n, t_n | h_{n-1}, t_{n-1})$$

for the joint probabilities of the particle heights must hold. If furthermore the involved noise has a Gaussian
distribution, the stochastic dynamics can be expressed by a Fokker–Planck equation for the time evolution of the probability density \( w(h, t) \):

\[
\partial_t w(h, t) = -\partial_h \left( D^{(1)}(h, t) w(h, t) \right) + \partial_h^2 \left( D^{(2)}(h, t) w(h, t) \right).
\]

(2)

Following the Itô definition cf. [20], the time evolution of the single particle elevation \( h(t) \) is given by the Langevin equation:

\[
\dot{h} = D^{(1)}(h, t) + \sqrt{D^{(2)}(h, t)} \Gamma(t).
\]

(3)

Here, \( D^{(1)} \) and \( D^{(2)} \) denote the drift- and diffusion coefficients and \( \Gamma(t) \) is the white noise with \( \langle \Gamma(t) \rangle = 0 \), and \( \langle \Gamma(t) \Gamma(t') \rangle = 2\delta(t - t') \). \( D^{(1)} \) and \( D^{(2)} \) are defined as the first and second order coefficients of the Kramers–Moyal expansion of the probability distribution of the vertical displacement \( h(t) \):

\[
D^{(n)}(h, t) = \frac{1}{n!} \lim_{\tau \to 0} \frac{1}{\tau} \left( \langle \hat{h}(t + \tau) - h \rangle^n \right)_{\hat{h}(t) = h}
\]

\[
= \frac{1}{n!} \lim_{\tau \to 0} \frac{1}{\tau} \int_{-\infty}^{+\infty} d\hat{h} \ p(\hat{h}, t + \tau | h, t)
\]

\[
\times \left( \hat{h}(t + \tau) - h \right)^n,
\]

(4)

where \( n = 1, 2 \). The crucial point of the stochastic analysis is that by means of (4) it is possible to estimate the coefficients \( D^{(n)} \) directly from given data in a parameter-free way. Thus knowledge of the deterministic part \( (D^{(1)}(h, t)) \) and the noisy part \( (\sqrt{D^{(2)}(h, t)} \Gamma(t)) \) of the stochastic process is obtained.

In the following we consider the dynamics after the first 100 s running time of the numerical model, after which the process can be assumed to be a stationary one [8] and thus the \( D^{(n)} \) coefficients become time independent. Furthermore, we want to note that, based on the knowledge of the Langevin equation, it is possible to reconstruct the noise \( \Gamma(t) \) from the data and to verify the Markov property of the dynamics and the Gaussian distribution of the noise \( \Gamma \) (see also [22,23]). We will demonstrate this later for our data.

Eq. (3) provides a method to characterise the segregational dynamics of individual particles. It is expected that the drift coefficient \( D^{(1)}(h, t) \) depends on the particle size and material parameters of a specific particle. Furthermore, \( D^{(1)}(h, t) \) can be interpreted to be related to an effective potential \( V(h, t) \), that is

\[
\dot{h} = D^{(1)}(h, t) = -\partial_h V(h, t).
\]

4. Analysis of vertical particle motion

Elevation time series of a “large” \( (r = 0.3) \) and a “small” \( (r = 0.18) \) particle in our hard sphere flow model were generated and evaluated according to Eq. (4). From now, normalised heights \( h^* = h/h_{max} \) for the particle elevation are used, where \( h_{max} = 2.28 \) for the large and \( h_{max} = 1.97 \) for the small particle.

Figs. 2 and 3 show the elevation time series, the elevation probability distribution, the drift- and diffusion terms \( D^{(1)}(h^*) \) and \( \sqrt{D^{(2)}(h^*)} \) and the effective potential \( V(h^*) \) of the motion of the large and small particle in the model flow. Omitting the noise term \( \sqrt{D^{(2)}(h, t)} \Gamma(t) \), the Langevin equation (3) becomes

\[
\dot{h}^* = D^{(1)}(h^*).
\]

This deterministic part of the heights dynamics will be taken as the basis of the following discussion.

At first the dynamics of the large particle is discussed. Considering \( D^{(1)}(h^*) \) in Fig. 2(c), one has to distinguish between ranges of \( D^{(1)}(h^*) > 0 \) and \( D^{(1)}(h^*) < 0 \). If \( D^{(1)}(h^*) = 0 \), fixed points are present, \( D^{(1)}(h^*) < 0 \) and \( D^{(1)}(h^*) > 0 \) correspond to downward and upward particle motion, respectively. For the large particle, stable fixed points with \( D^{(1)}(h^*) = 0 \) are situated at \( h^* = 0.37 \) and \( h^* = 0.53 \). At \( h^* = 0.41 \), there is a saddle point (or repulsive fixed point). These stable fixed points correspond to the increased probabilities for the large particle as shown in Fig. 2(b). The saddle point at \( h^* = 0.41 \) between the stable fixed points is represented by a local minimum in the particle localisation probability density.

The plot of potential \( V(h^*) \) (Fig. 2(d)) corresponding to \( D^{(1)} \) shows two local minima at the elevations of the stable fixed points of the large particle elevation dynamics. The particle elevation is shifting between the two potential minima corresponding to different flow layers. Transitions from one to another potential minimum are induced by noise (i.e., fluctuations in the flow). The potential barrier corresponds to the repulsive saddle point at \( h^* = 0.41 \).

For the small particle, \( D^{(1)}(h^*) \) hardly exceeds zero except for some small fluctuations but becomes less than zero for \( h^* > 0.4 \) (Fig. 3(c)). The increasing er-
errors in $D^{(1)}(h^*)$ for $h^* > 0.5$ are due to poor statistics: the small particle elevation very rarely exceeds $h^* = 0.5$.

In correspondence to the structure of $D^{(1)}(h^*)$, we find a broad minimum in the range $h^* < 0.4$ for the potential $V(h^*)$, from which in connection with the unstructured noise given by $D^{(2)}(h^*)$, we conclude that the elevation dynamics of the small particles can be described by a constant noise driven motion in a metastable regime. This feature is also reflected in the quite unstructured probability distribution. The weak maxima in the elevation probability are periodic in the diameter of small particles corresponding to layering of small particles near the ground. However, the small particle predominantly is situated in the ground layer. Accordingly, the elevation dynamics in the lower (small) particle layers is only weakly reflected in the plots of $D^{(1)}(h^*)$ and $V(h^*)$.

After the discussion of the meaning of the drift and diffusion terms $D^{(1)}(h^*)$ and $D^{(2)}(h^*)$ for the dynamics of small and large particles, we now turn to the question whether the underlying elevation dynamics is Markovian. As described above, we reconstruct the noise from the time series by Eq. (3) using $D^{(1)}(h^*)$ and $D^{(2)}(h^*)$ which have been extracted directly from the data (Eq. (4)). In Fig. 4(a), the extracted noise signal for the large particle motion is shown. We find that the autocorrelation (see Fig. 4(b)) decays very fast and that the noise distribution is Gaussian with mean value of $\langle \Gamma(t) \rangle = 0.03 \pm 0.07$ (Fig. 4(c)). These two features provide evidence that the dynamics of $h(t)$ is Markovian.

Note that the Gaussian distribution of $\Gamma(t)$ implies that the Kramers–Moyal expansion of the probability distribution of the vertical dynamics $p(h^*)$ is cut after the second order term and therefore Eqs. (2) and (3) are a complete description of the observed dynamics.

5. Conclusion

We have demonstrated that the effect of inverse grading can be reproduced in the context of a simple hard sphere model of rapid granular flow in the inertial regime. Inverse grading can be interpreted as an overall statistical effect of all the particles participating in the granular flow.

The stochastic nature of inverse grading in a hard sphere grainular model flow is proven by analysis of the deterministic and the noise contributions of the dynamics of vertical motion of individual particles. We found evidence that the observed inverse grading is caused by the deterministic component of the reconstructed effective stochastic process, which may be considered as a macroscopic dynamics of the granular flow.

In this sense, the application of the stochastic analysis to the description of inverse grading generated by direct numerical modelling may be interpreted as a step from a purely micromechanical point of view towards a stochastic based overall view of the granular flow behaviour.

Stochastic analysis of particle elevation time series provides a simple deterministic description of single particle elevation dynamics. Interpreting the drift coefficients $D^{(1)}(h^*)$ as deterministic dynamics underlying the apparently disordered vertical particle motion, it is, in principle, possible to replace costly direct
numerical simulations of segregational behaviour of granular media by an effective segregational dynamics, which may be parametrised with the particle size. This may have practical implications, as a method is now available to predict segregational behaviour of a given multidisperse granular material from the analysis of single particle elevation times series.

Acknowledgements

This work has been part of the project “burial prophylaxis with avalanche airbags” which was funded by the Schweizerische Unfallversicherungsanstalt (SUVA), Luzern.

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