

Molecular dynamics simulation of powder fluidization in two dimensions

J.A.C. Gallas^{a,b}, H.J. Herrmann^a and S. Sokołowski^{a,c}

^a*Höchstleistungsrechenzentrum, KFA, W-5170 Jülich, Germany*

^b*Laboratório de Óptica Quântica da UFSC, 88049 Florianópolis, SC, Brazil*

^c*Department of Theoretical Chemistry, MCS University, 20031 Lublin, Poland*

Received 22 July 1992

We report model calculations of a fluidized state in a two-dimensional packing of spherical beads subjected to vertical vibrations as recently experimentally studied by Clement and Rajchenbach. Using molecular dynamics we calculate the density field and the velocity distributions of the beads. We discuss the concept of fluidization and propose new ways to characterize it.

The rheology of granular material like sand, powder or pills provides many scarcely understood, astonishing phenomena [1]. Examples are the so-called “Brazil nut” segregation [2–4], heap formation under vibration [5–8] and the density waves emitted from outlets [9]. All these effects seem to eventually originate in the ability of granular materials to form a hybrid state between a fluid and a solid. Reynolds [10] introduced the concept of dilatancy, the critical density below which “fluidization” sets in, based on the principle that density is the main factor controlling the rheology. Under density gradients or fluctuations, granular material seems therefore capable of changing from solid- to fluid-like behavior giving rise to the aforementioned mysterious effects. A particularly relevant experimental set-up to study this fluidization is putting sand on a vibrating table or on a loudspeaker [5–8, 11–14]. Under gravity the sand jumps up and down and although kinetic energy is strongly dissipated, collisions among grains reduce its density thereby allowing it to flow. This kind of fluidization is different from the so-called “fluidized beds” [15,16] in which bubbles of air or another fluid are pushed through the granular material.

In a recent paper Clement and Rajchenbach (CR) [11] report experimental observations of a “fluidized” state in a 2D vertical packing of steel spheres submitted to vertical vibrations. They shake periodically (at $f = 20$ Hz) 300 steel beads inside a trapezoidal cell built with side walls making 30° with

respect to the vertical axis. Position and velocities of the particles were obtained by photographing the system periodically and then averaging over 15 snapshots taken at a given constant phase φ . Velocities were obtained from averages over a time interval τ around the phase φ . From a plot of the density of particles they argued fluidization to occur in the upper region of the packing. The measured density of particles showed a curious effect: the mean density was found not to depend on the phase of the vibration, implying the appearance of a steady state preserving the density profile at all times, independent of the up and down collective motion. From plots of the average velocity components they concluded that the mean velocity of the particles does not depend significantly on their height inside the container, if a few particles undergoing ballistic flight above the packing are neglected. However, important velocity fluctuations were observed for heights in which the density profile significantly varies. In fact they observed velocities at different phases φ to fluctuate, although the overall density field remained always constant.

The main purpose of this letter is to see whether we are able to reproduce numerically the phenomena observed by Clement and Rajchenbach [11], to quantify the concept of fluidization and to check if the relevant parameter for fluidization is given by Af^2 where A is the amplitude of the vibration [12]. The working tool that we use for this purpose is molecular dynamics (MD) [17,18]. In fact MD has been used already for granular media to model segregation [4], outflow from a hopper [19], shear flow [20] and convection cells [21].

Our model includes the fact that dissipation of energy occurs via inelastic interparticle collisions as well as via collisions of the particles with the walls. The molecular mechanism of energy dissipation is very complicated and can obviously not be treated on the same time and size scales as the collisions between beads. The geometry and dimensions of the container were chosen identical to those used in the experiments of Clement and Rajchenbach [11]. The two-dimensional box containing the beads was delimited by two different types of walls: those forming the trapezoidal delimitation seen in fig. 1, and those that we will refer to as “parallel walls”, parallel to the plane of the figure. The experimental distance between the two parallel walls was 3.0 mm. Our trapezoidal line was built of spherical particles (vertices) identical to the beads and separated from one another by $\sigma = 1.55$ mm. Altogether, the beads were subjected to three forces: interparticle repulsion, a 10 m/s^2 acceleration due to gravity and friction forces. We assume that the spherical particles interact according to Hooke’s law, namely, that the repulsive interparticle potential energy is given by

$$u(r) = \begin{cases} \frac{1}{2} Y(d-r)^2 & \text{for } r \leq d, \\ 0 & \text{for } r > d, \end{cases} \quad (1)$$

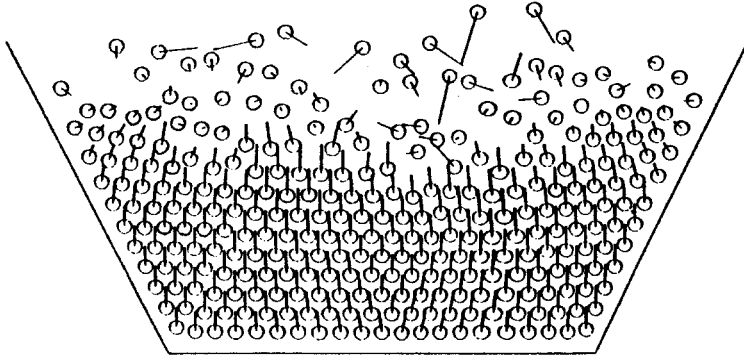


Fig. 1. The center of the circles are the positions at $\varphi = 0$ whereas the end of the lines display the positions 15 ms later. A few beads flying too high are not shown.

where Y is the Young modulus and $d = 2.99$ mm is the diameter of the beads, as in the experiments. This same equation is used to describe interactions between beads and vertices of the trapezoidal line. Eq. (1) is of course only valid for relatively small forces (linear elasticity). We did not take into account eventual Hertzian contacts, which in two dimensions would imply an additional logarithmic prefactor and in three dimensions would give an exponent of $5/2$ in eq. (1). These effects only come into play for ideal spheres and we might assume here for simplicity that locally the spheres are rather flattened.

Three types of friction exist in the present experiment: friction due to frontal bead–bead collisions, to collisions between beads and the trapezoidal line and, lastly, to the confining parallel walls. The first two types of friction were assumed to contribute similarly to the energy dissipation: proportional to the relative velocity of the colliding particles. To reduce the number of parameters, the constant of proportionality was always considered to be the same. The effect of the last type of friction was considered in exploratory simulations but found not to contribute significantly to the fluidization. Therefore we will ignore it.

The equation of motion of the i th bead at horizontal position x and at height z is then given by

$$\frac{d\mathbf{r}_i}{dt} = \sum_j \left(-\frac{1}{m} \nabla_i u(|\mathbf{r}_i - \mathbf{r}_j|) - \mathbf{a}_{ij} \right) - \mathbf{g}, \tag{2}$$

where $\mathbf{r} = (x, z)$ and the summation is performed over all interacting centers (beads and wall vertices). The components of the friction \mathbf{a} acting when the particles are in contact are given by

$$(a_{ij})_x = -c|\dot{x}_i - \dot{x}_j| \operatorname{sgn}(\dot{x}_i) \quad \text{and} \quad (a_{ij})_z = -c|\dot{z}_i - \dot{z}_j| \operatorname{sgn}(\dot{z}_i), \tag{3}$$

and the gravity g is parallel to the z -axis. The vertical periodic movement of the container was modelled by $z(t) = A \sin(2\pi ft)$. In the experiment, $A = 2.5$ mm and $f = 20$ Hz [22].

The equations of motion have been solved numerically by using classical predictor–corrector methods [17,18]. The suitable parameters to model the experiment were found to be $Yd/m = 20\,000$ m/s² and $c = 300$ s⁻¹. The relatively small value of Y was taken to allow for the use of a more convenient time-step for the numerical integration. This is not critical for the results of the simulation: We have made some test runs with a value of Y two orders of magnitude larger and found qualitatively the same results. Having selected Y , we sought an interval of c values such that the experimental results could be fitted well. In fact, the simulations show that a change of 20% in c does not modify our results very much. Our simulations had a time step of $\Delta = (4000f)^{-1}$ and the inner, vectorizable loop of the program ran at 170 MFlops on one Cray-YMP processor.

We started simulations from a random distribution of beads inside the cell, letting them fall freely under gravity. The system was allowed to evolve until the averaged squared velocity per bead was smaller than 10^{-8} m²/s². After that we simulated the shaking by letting all wall vertices undergo harmonic oscillations as described above. By comparing snapshots taken at different phases $\varphi = 2\pi ft$ it is possible to reconstruct the motion of the beads during a full cycle of the shaking. Fig. 1 is intended to be our equivalent to fig. 1 of CR. The dots represent positions of the spheres at $\varphi = 0$ while the end of the line segments indicate where the particles are located at a time $t = 15$ ms later. One may easily realize that while the movement of our spheres is rather symmetric with respect to a reflection about a vertical line passing through the center of the cell, the corresponding experimental picture obtained by CR is not so. We attribute such differences to small uncontrollable non-uniformities in the experimental set-up. Fig. 2 shows local densities along the z -axis, evaluated at different phases as described in the experimental paper. A full shaking period in the experiment took 50 ms [22] and the time averages considered by CR were over 15 ms, i.e. slightly longer than a quarter-period. Our curves were obtained by averaging the local density over the 15 ms following each phase φ and over 30 shaking cycles after discarding 30 “transient” cycles. For spatial averages, it was important to place the horizontal axis of the grid system used to perform averages as passing through the bottom of the oscillating container. As can be seen from this figure, our model correctly reproduces the experimental behaviour of the beads, producing the same smoothly varying density profile as a function of the height. Some ballistic flights were also observed in our simulations.

Fig. 3 presents our results for the averaged v_z and v_x velocities averaged

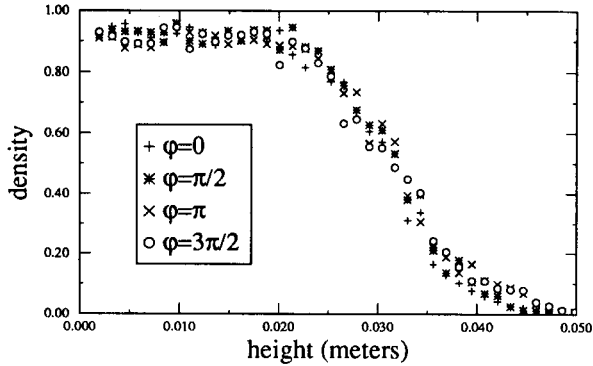


Fig. 2. Local density, normalized by the solid density, as a function of the height z for different phases of the vibration for $A = 2.5$, $f = 20$ Hz averaging over 30 shaking cycles after having discarded 30 cycles in order to reach steady state.

exactly in the same way as the local density. The first point to note is that, as in the experiments, the absolute value of v_x is substantially smaller than v_z , in conformity with the symmetry of the driving force.

Since for all phases and over many cycles of the driving force the beads in the bulk locally maintain their regular hexagonal-lattice-like arrangement, one would think that its properties are more solid-like inside the bulk, while the few upper layers without translational symmetry behave more like a fluid. To check whether the present model is at all able to display a transition from a solid- to a fluid-like state we performed additional simulations, varying both frequency and amplitude of the oscillations. A further objective in doing this was to check whether $Af^2/g \geq 1$ characterizes the onset of fluidization. So, in

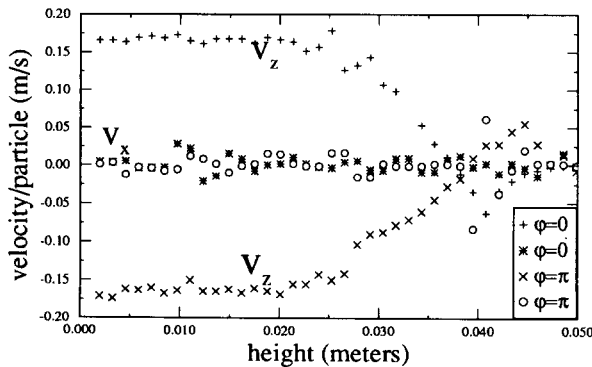


Fig. 3. Average bead velocities v_x and v_z per particle as a function of the height z at two different phases: $\varphi = 0$ and $\varphi = \pi$. The parameters are as in fig. 2.

the simulations we calculated two additional quantities to characterize the state of the system, namely, the time-dependence of the vertical position of the center-of-mass of the beads $\langle z \rangle$ and the mean square displacement of individual beads as a function of time. To access the relative mobility of pairs of beads in the ensemble for each particle i we selected its nearest neighbour j and the respective distance r_{ij}^0 . Then, for each subsequent time t we evaluated the quantity

$$R(t) = \frac{1}{Nt} \sum_{i=1}^N \sum_{\tau=0}^t (r_{ij}^{\tau} - r_{ij}^0). \quad (4)$$

For a solid each bead is confined to a cage formed by its neighbors and $R(t)$ should be a constant of the order of the lattice constant. If however the behavior is fluid-like, each bead will perform essentially a Brownian motion and $R(t)$ should be asymptotically proportional to $t^{1/2}$, defining as proportionality constant a diffusivity D .

We recorded the trajectory of a selected “tracer” particle, and monitored its motion as time evolved. Fig. 4 shows two situations with different amplitude A and frequency f , one with solid-like bulk (figs. 4a and 4c) and the other with a fluid-like bulk (figs. 4b and 4d). In figs. 4c and 4d we see 8000 positions of the tracer particle recorded every 50 time-steps, for a particle that was initially located roughly in the center of the packing. In the first case the tracer particle remains confined to a very small region while in the fluid-like case the trajectory seems to explore the entire box. The distinction between solid- and fluid-like situations in the bulk also becomes obvious from the snapshots of figs. 4a and 4b. It is important to note that both situations of fig. 4 correspond to the same value of Af^2 . This means that Af^2 is not a good scaling variable even close to the onset of fluidization.

Fig. 5 shows more quantitative evaluations of the degree of fluidization. In fig. 5a we see how the distance between pairs of beads, namely the $R(t)$ defined in eq. (4), increases in time. We see that after a transient of slower growth, $R^2(t)$ increases linearly in time for large times in all the five different cases considered. The asymptotic slope defines the diffusion constant. The five curves have different amplitudes and frequencies but in three of them, namely (case a), (case d) and (case e), the product Af^2 is the same. Clearly, however, the diffusion constants are very different in the three cases, showing again that the fluidization properties are not determined by the simple formula Af^2 . It is also interesting to note that none of the five curves in fig. 5a seems to go to a constant as predicted for the bulk of the solid-like case. The reason is that the data of fig. 5a are averages over all pairs of particles that were initially close neighbors and as seen in fig. 4a the solid-like bulk is surrounded by layers of more mobile particles.

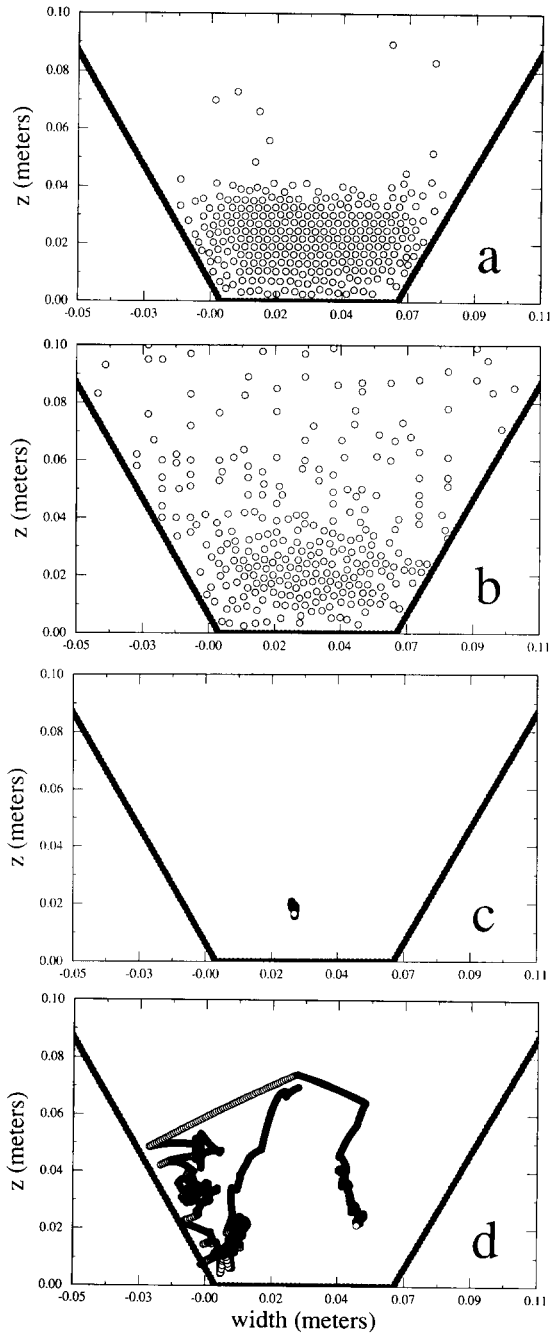


Fig. 4. Comparison of solid- and fluid-like behavior. (a) and (b): lower part of the system after shaking (see text); (c) and (d): trajectories of test particle in each situation. The walls are displayed at $\varphi = 0$. (a) and (c) correspond to $f = 60$ Hz and $A = 4d/3$; (b) and (d) to $f = 40$ Hz and $A = 3d$. In both cases have the same value of Af^2 .

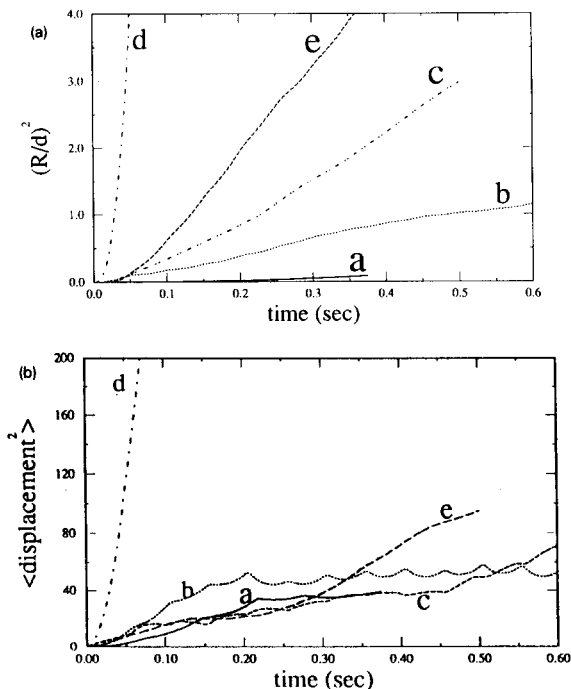


Fig. 5. (a) The square of $R(t)$ as defined in eq. (5), and (b) the mean square displacement of a tracer particle as a function of time for different frequencies and amplitudes. The data are averaged over all particles. Legend: (case a) $f = 80$, $A = 3/4$; (case b) $f = 20$, $A = 2.5/2.99$; (case c) $f = 20$, $A = 3$; (case d) $f = 40$, $A = 3$; and (case e) $f = 60$, $A = 4/3$, all frequencies in Hz and amplitudes in units of d . For case a, case d and case e the quantity $Af^2 = 14.35 \text{ m/s}^2$ is the same.

Using the same nomenclature for the five different cases we show in fig. 5b the mean square displacement of a tracer particle as a function of time. Again violation of the simple Af^2 scaling is observed. Clearly case d sticks out from the other cases and in fact one also observes a qualitative difference comparing fig. 4a (case e) and fig. 4b (case d). So it seems that fig. 5b can be used to distinguish if a solid-like bulk exists or not. We also see that in some situations (e.g. case b) the packing follows quite closely the motion of the vibrating plate which seems yet another way of characterizing a solid-like behaviour.

In conclusion we have numerically investigated aspects of the fluidization of a granular material. To see whether our MD techniques properly model realistic situations, we reproduced two-dimensional experiments performed by Clement and Rajchenbach and found good agreement in the density and velocity profiles. We considered situations with different frequencies f and amplitudes A of the vibration and found clear evidence against an eventual scaling of statistical properties with Af^2 . The concept of fluidization itself is

also ambiguous – at least one can define qualitatively different types of fluidization. At very high frequencies any tracer particle performs essentially a random walk. In this case the average height of the packing can be several times the height of the packing at rest. At lower frequencies a solid like bulk appears in which a tracer particle is trapped and this bulk is surrounded by more mobile particles. At even lower frequencies the average height of the packing follows the oscillations of the vibrating plate. In all these cases however one can define an average diffusion constant that is not zero.

The present study sheds more light on the problems connected with fluidization although several important ingredients have not been taken into account here: particles have rotation, Coulomb (dynamic) friction and static friction, the particles are not perfectly circular and identical and, finally, most experiments are of course three dimensional. Molecular dynamics seems to be a good tool to explore these questions further. Indeed, it has been shown recently that with the same model as presented here, i.e. even without solid friction, it is possible to obtain even in two dimensions the famous convection cells that appear on vibrating tables [21]. For granular media also continuum equations of motion [23], a thermodynamic formalism [24] and cellular automata [25] have been formulated and it would certainly be interesting to explore the effects of fluidization discussed in this paper within these theories.

We thank E. Clement, J. Rajchenbach and G. Ristow for fruitful discussions. J.A.C.G. is a senior fellow of the CNPq (Brazil).

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