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Hard sphere packing on an inclined plane

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Abstract. Deposition of monodisperse hard spheres onto an inclined surface has been investigated. The process of random sequential deposition of particles in the downwards vertical direction was simulated on a computer. It was found that the solids volume fraction of the resulting aggregate is an increasing function of the angle of inclination of the surface to the horizontal.

1. Introduction

Many studies of the packing of hard spheres have been undertaken [1–4]. Here the effect of the angle of the plane on which the packing is built is investigated. The motivation for the simulation was provided by cross-flow cake filtration experiments carried out by Mackley and Sherman [5]. Their work involved filtration of 100 μm polyethylene particles in a neutrally buoyant Newtonian liquid, both with and without a cross-flow velocity perpendicular to the direction of the filtration flux. Results showed that cakes grown in static filtration (no cross-flow) have a lower solids volume fraction than those grown in cross-flow filtration. These results suggest that the packing of an aggregate formed by deposition will be affected by the angle at which incoming particles approach the aggregate surface. The object of this work is to try to investigate these findings by simulating on a computer the vertical deposition of monodisperse hard spheres onto a base inclined at an angle ϕ to the horizontal, and measuring the solids volume fraction of the resulting aggregate as a function of ϕ. This work is not designed as a complete model of aggregate formation in cross-flow filtration, but seeks to reproduce some of its main features in a simplified situation. The purpose of the simulations is to determine whether the packing fraction of an aggregate depends on the angle of approach of incoming particles to the aggregate surface. The simulations deal with the simple case of sequential deposition which corresponds to a filtration experiment where the filtrate flux has a low solids volume fraction.

2. Numerical simulations

The algorithm used to generate the aggregate is the same as that of Visscher and Bolsterli [1], the only difference being that the base layer is at an angle ϕ to the horizontal. A coordinate system (x, y, z) is set up with the x and y axes horizontal and the z axis pointing vertically upwards. Rotation of the (x, z) axes about the y axis by an angle ϕ leads to a coordinate system (x', y', z') with (x', y') in the plane of the base and z' perpendicular to the base

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(see figure 2). The system consists of a hexagonally close-packed (HCP) base layer of 105 spheres of unit radius, having base dimensions of $18\cos(\phi) \times 10\sqrt{3}$. Periodic boundary conditions are employed in the x' and y' directions. The particles are added sequentially, each particle being dropped from above the base layer at a point in the x–y plane chosen at random. The point of first contact with a sphere already forming part of the aggregate is calculated. The deposited sphere then rolls in contact with this sphere until it either contacts another sphere, or falls off the first sphere and undergoes free-fall once more. When in contact with two spheres the deposited sphere rolls, touching both spheres until it either ceases to contact one of the spheres and rolls in contact with the other, or it contacts a third sphere. If the deposited sphere contacts three others, a test is performed to see whether it is in a stable position. Stability occurs when the centre of the deposited sphere is above the triangle joining the centres of the three supporting spheres. If the sphere is unstable it rolls in contact with the two supporting spheres which provide the steepest descent for the deposited sphere. If it is stable it is added to the aggregate. In this program the assumption is made that once a sphere becomes part of the aggregate its position remains fixed throughout the rest of the simulation. In making this assumption the grains are effectively considered to be infinitely rough (i.e. they have an infinite coefficient of friction).

The HCP layer was used as the base layer for simulations at angles up to a critical angle ϕ_c ($= 22.21^\circ$). However, for $\phi > \phi_c$ the HCP layer contains no stable sites and had to be artificially roughened by *sticking* another layer of spheres at random onto the HCP layer. This new layer was used as the base layer for all of the simulations at any particular angle.

One way to test the program is to repeat the simulations with a different sized base, and also a base with a different aspect ratio. Test simulations were carried out at an angle of inclination of 20°, with a system with base dimensions of $30\cos(20^\circ) \times 14\sqrt{3}$. The volume fraction of this larger system was 0.5824 ± 0.0005 (average of 10 simulations), in good agreement with the results for the smaller system. Another obvious test is to compare results from simulations performed with ϕ set to zero, with the results of previous simulations of hard sphere deposition onto a horizontal base [1, 2]. The volume fraction obtained with $\phi = 0^\circ$ was 0.5812 ± 0.0003, which agrees well with the results of Visscher and Bolsterli [1] and Jullien and Meakin [2] who obtained volume fractions of 0.582 and 0.5815 ± 0.0002, respectively, for deposition onto a horizontal base. A final measure was to examine each packing for overlapping spheres. All pairs of spheres were checked to make sure they satisfied the relationship $R^2 > 3.999$, where R is the centre–centre separation of the two spheres. This procedure ensures that none of the aggregates generated have an error in the packing fraction, due to overlapping spheres, greater than 0.0002.

The volume fraction was measured as a function of angle of inclination to the horizontal. This was done by calculating the volume of a periodic cell occupied by spheres, between two planes parallel to the inclined base. The height of these two planes must be chosen to eliminate from the calculation of the higher volume fraction near the HCP base layer and the lower volume fraction near the aggregate surface. This was done by increasing the height of the plane at lower z' until the average value of the volume fraction was no longer falling, and reducing the height of the plane at higher z' until the average volume fraction was no longer rising. In each simulation the presence of a large region within the bulk of the aggregate where the packing fraction remained constant was checked. The existence of such a region, along with the independence of packing fraction on the size or aspect ratio of the base layer, removes any ‘finite system size’ effects from the calculation of the packing fraction. At each angle 10 simulations were performed, each using 4000 spheres. To simulate the deposition of 4000 spheres took approximately 40 minutes CPU time on an IBM3084 computer.

3. Results

Figure 1 shows that the volume fraction increases with increasing ϕ, which is in qualitative agreement with Mackley and Sherman's findings that cross-flow filtration results in cakes with higher resistances than cakes grown in the absence of any cross-flow. The error bars plotted in figure 1 are the random errors in the simulations at each angle. These errors seem surprisingly small considering those of Jullien and Meakin [2] for a larger system; however, they were calculated in a reasonable way (as the standard errors of 10 simulations) and there appears to be no obvious reason to doubt their voracity. Applying the Kozeny–Carman equation [6] (which relates cake resistance R to void fraction ε ($R \propto (1-\varepsilon)^2/\varepsilon^3$)) to these results gives the ratio $R(\phi = 45^\circ)/R(\phi = 0^\circ) = 1.06$, which is much smaller than Mackley and Sherman's finding that the resistance of cakes formed in cross-flow filtration was three times larger than of cakes formed in static filtration. However, important differences exist, such as local variations in the velocity field at the aggregate surface which can result in particles being stabilized by forces acting in directions which differ from that expected by consideration of the mean filtration and cross-flow velocities. This suggests that in the cross-flow filtration experiments packings can be built up even when the cross-flow velocity is much larger than the filtrate flux. This contrasts with the simulation, in which stable packings could not be generated above a maximum angle of inclination $\phi_{\max}$. The value of $\phi_{\max}$ found in the simulation was approximately 45°. This is not to say that packings *cannot* be built up on bases inclined at $\phi > 45^\circ$. Wilkinson [7] calculated the angle of repose for sequentially deposited monodisperse spheres at 58°. However, Wilkinson's simulation and the one presented here contain differences. In Wilkinson's work the angle of repose was calculated by building up a pyramid structure of spheres on a rectangular base until no stable sites remained, the final resting place of each sphere being chosen at random.

A number of different base layers were tried at $\phi = 50^\circ$, but none could sustain a large stable configuration: after addition of a small number ($\sim$500) of particles there were no

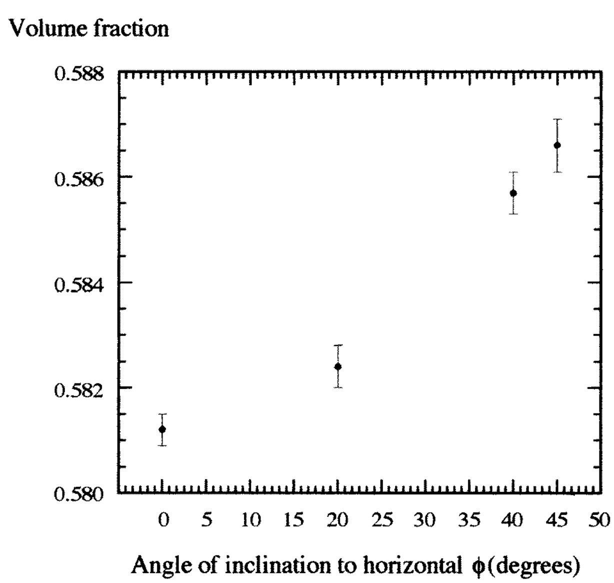

Figure 1. Volume fraction versus angle of inclination of plane to the horizontal.

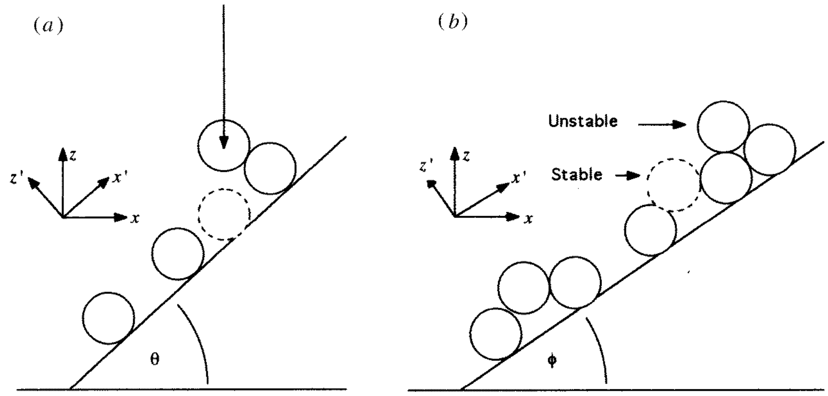

Figure 2. Schematic representation of the availability of stable sites. (*a*) Spheres stick at the first point of contact. Sites which would be available at lower angles of inclination θ, are screened by neighbouring spheres. (*b*) Spheres roll to the final resting place. Sites which would be stable at lower angles of inclination but would result in less compact structures, become unstable at higher angles of inclination ϕ.

stable sites left. This was investigated further by depositing a maximum of 4000 spheres onto the HCP base layer using an algorithm identical to Wilkinson's. These results can be summarized by saying that below 45° one can add any number of new spheres to an existing packing without causing the number of stable sites to go to zero, and that above 50° this is not possible because any existing packing will have all its stable sites filled by the addition of a (small) finite number of particles. At intermediate angles there is a probability between one and zero that a stable packing of N spheres can be built up. This probability will be a decreasing function of N as well as of the angle of inclination.

The results shown in figure 1 can be contrasted with results obtained by Jullien and Meakin [2] who used a model in which sequentially deposited spheres stick to the aggregate at their first point of contact. Spheres following vertical trajectories were deposited onto aggregate surfaces inclined at an angle θ to the horizontal. The volume fraction of the resulting aggregate was a *decreasing* function of θ. The reason for this behaviour is illustrated in figure 2(*a*). The packing fraction will be larger if on average newly deposited balls come to rest with lower values of z'. One can see that, for larger values of θ, trajectories which would lead to lower values of z' are screened by neighbouring balls. On average the size of gaps through which balls must fit to obtain lower values of z' reduces with θ. The situation for balls which do not stick on contact, but roll to their final resting place is very different. This can be explained by considering what happens to the stable sites on the surface of an aggregate as one increases the angle of inclination ϕ (see figure 2(*b*)). Stable sites having a higher value of z' which exist for lower values of ϕ, cease to be stable at higher values of ϕ leaving sites at lower values of z' only. Therefore, although the number of stable sites decreases with ϕ, the sites which remain will result in an aggregate having a packing fraction which increases with ϕ.

4. Conclusions

The deposition of monodisperse hard spheres onto an inclined plane has been simulated numerically. The packing fraction of the resulting aggregates increased with the angle of inclination of the plane to the horizontal. This is in qualitative agreement with Mackley and Sherman's finding that aggregates grown in cross-flow have a larger resistance than aggregates grown in the absence of any cross-flow. These results can be contrasted with those obtained for ballistic deposition [2], in which particles stick to the aggregate at their first point of contact, where the packing fraction is a decreasing function of the angle of inclination to the horizontal.

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