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The Packing Problem: Effect of a Packing Process on Granular Material

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Contents

1 Introduction

Granular materials appear in almost every industrial manufacturing process. Primary materials such as silicon or polymers are used in a granular form or the end product itself is a granular material such as M&M®'s candies. For an advanced processing of granules a detailed knowledge of the material characteristics is required [8]. Questions to be asked are, how dense one could pack a specific kind of granules or, what kinds of actions force a packing of granular material to change its characteristics' values such as the density or the orientational order? The effect of even a small force on granular materials can change these values which might cause a totally different behavior of the granular materials [7]. During the transportation and processing of granules force effects occur all the time which results in a so called packing process which increases the density of the granular material and changes other characteristics.

The investigations presented start with the way granular materials are stored: in a packing of granular materials the initial density, called the *random loose packing (RLP)* is influenced by the geometry of the box in which the packing is observed[15]. To get a *RLP* into the state of a random close packing *(RCP)* the packing has to go under a packing process, e.g. shaking. In this thesis the wall effect is discussed as well as the relevant parameters for the *RLP* and the packing process itself.

A Short History of the Packing Problem

"How should we arrange objects to pack them as tightly as possible, making best use of all the available space?" The packing problem has been studied systematically since the 17th century [12]:

Isaac Newton (1642-1727): maximal coordination number of a sphere packing is 12 in a 3D Euclidean space;

Johannes Kepler (1571-1630): Kepler conjecture (1611): the densest packing of identical spheres is achieved in a face-centered cubic structure, with a packing fraction of 74%;

Carl Friedrich Gauss (1777-1855): publication of a partial solution in 1831; Gauss proved that the Kepler conjecture is true if the spheres have to be arranged in a regular lattice;

David Hilbert (1862-1943): included Kepler conjecture in his list of twenty three unsolved problems of mathematics in 1900;

Thomas Hales, University of Michigan: first comprehensive modern computer simulation of packing structures in 1998.

Now: How can one pack a packing using the most effective way?

2 Definitions and Notations

2.1 General

packing A packing consists of a specified amount of particles in a box. The particles are well defined by their basic shape S, aspect ratio a and friction coefficient F.

box We consider a box as a three dimensional geometrical body with the basic shape of a cylinder, a height h and an average diameter D. The box is filled with particles to a certain filling height H.

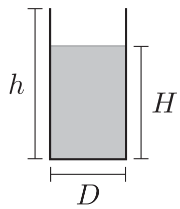


Figure 1: Box dimensions

RLP When a packing is built by filling the particles in the box randomly the packing is in the state of a *random loose packing*. Parameters to consider beside the particle parameters are the filling amount, the filling rate and the box characteristics itself.

RCP A maximal compacted *RLP* is called *random close packing*. The characteristics of a *RCP* are independent on compacting parameters and friction between the particles and box walls. Figure 2 shows the difference between a *RLP* and a *RCP*.

packing process If a packing is compacted it has to go under a packing process. A packing process causes a higher density of the packing and can be achieved by shaking or vibrating the box in specified directions. A packing process is called finished if the packing has reached the state of a *RCP*.

wall effect Under certain circumstances the box geometry influences the density and other characteristics of a packing in the state of a *RLP* and during the packing process directly, which is called the wall effect.

2.2 Characteristics of a Packing

2.2.1 Density

The fraction of space occupied by granular particles in a box is referred to the density p.

$$p = \frac{V_S}{V_T} \tag{1}$$

where V_S is the space occupied by granular particle and V_T the total box volume:

$$V_T = \frac{1}{4} D^2 \pi \cdot H \tag{2}$$

Figure 2: Comparison between *RLP* and *RCP*

Measurement of the Density

A scale was recalibrated after putting the empty box on it. After the determination of the average weight m_p and dimensions of a single particle, the box was randomly filled to create a *RLP*. By dividing the weight of the box content m_b by the average weight of a single particle we obtained the numbers of particles N inside the packing:

$$N = \frac{m_b}{m_p} \tag{3}$$

This number multiplied by the average particle volume V_S represents the space which is actually occupied by the particles. Now it possible to calculate the density of the *RLP* (see equation 1).

Measurement of the Density during the Packing Process

As mentioned before, the density increases during a packing process which decreases the actual filling height H used for the calculation of V_T in equation 2. A photo analysis was used to determine the density of granules in a box because determining H manually after every single box movement is too imprecise and would take too much effort. A simple approximation by utilizing an image editor would be too inaccurate. To obtain the best approximation for H a program (listing 1) summed the greyscale values for every row and calculated the average value after a threshold operation was applied to the picture [13].

```
// compute row average and save
reduce(imageWarp, lines, 1, CV_REDUCE_AVG, CV_32FC1);
fs << num << "\t";
for( int j=0; j<lines.rows; j++ ){
      fs << lines.at<float>(j) << "\t";
}
fs << endl;
cout << num << ", " << flush;
```

Listing 1: Picture Analysis to determine H

From the row averages a good approximation for H was possible. The program is written in C++ and works with the open source library OpenCV [3] which provides many useful functions for image editing.

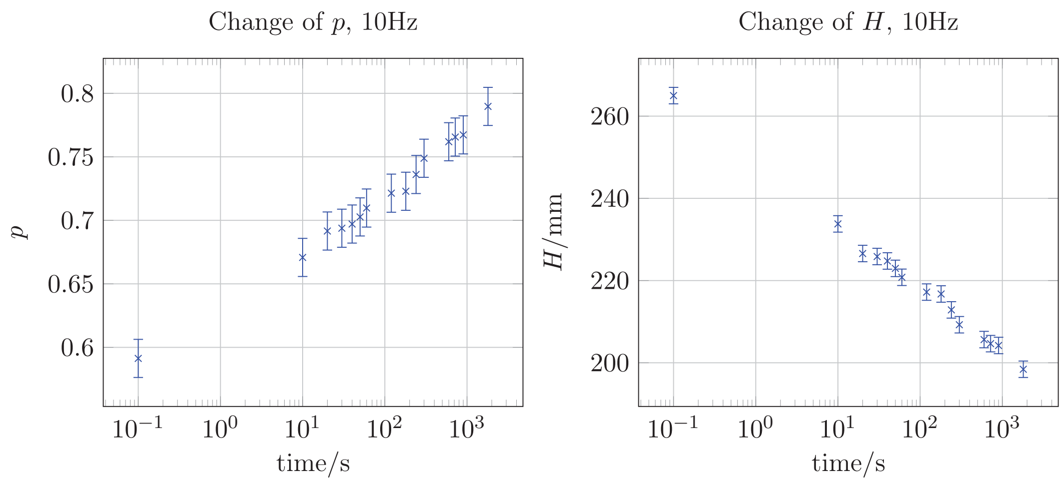


Figure 3: Actual filling height H as a measurement for the density p

Due to the fact that the actual filling height H is indirectly proportional to the density inside the packing the density change can be easily represented by the change of H as seen in figure 3 .

2.2.2 Coordination Number

A single particle in a packing has direct neighbors which are defined by a physical contact. The neighbors of all particles summed up divided by the numbers of particles inside describes the average coordination number of a packing.

Measurement of Coordination Number

Measuring the average coordination number of a packing is difficult. Counting the physical particle contacts by hand is nearly impossible because every movement of a particle, which would be necessary, would cause a different orientation of the particles which has an influence on other characteristics. A picture analysis is also not possible because of obvious reasons (see figure 4). There is a method of using a computer tomograph to get a 3D image of the whole packing which makes software based contact counting easy [9]. Due to the fact that a computer tomograph was not available for this research, a more pragmatic method was used: the packing was created and immediately afterwards filled with common liquid gelatine which set a few hours later. The resulting solid consistency of the packing allows movements of single particles without destroying the remainder of the original packing configuration.

2.2.3 Orientational Order

Particles can be orientated differently. The orientational order of a packing is obtained by the distributions of the centers of mass and the two defining angles of the particles.

Measurement of Orientational Order

A few measurements were taken by analyzing pictures but due to the missing values for the inner part of the packing there was a focus on literature. The same method

Figure 4: Particles held together with gelatine

as it was used for the determination of the coordination number was tried but there were no considerable results taken.

2.3 Error Estimation in the Experiments

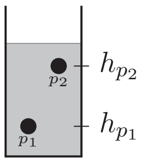
This thesis focuses mainly on experiments the author performed herself. The data analysis of the results always includes an error estimation which allows one to determine to what extent the experiment is significant. There was account taken of errors in measurement and analysis tools as well as statistical errors. The errors vary in some experiment even if the same property is investigated. This is due to the fact that some parameter variations cause different changes in the property to be investigated. That is why a faster and more effective analysis with some loss of accuracy was sometimes used for practical reasons. It has to be pointed out that a certain lack of precision did not falsify the overall purpose of the experiments. A reference to a non existent validation or contradiction of a theory in an experiment due to measurement errors always implies that even though the most accurate analysis method was used the errors were to high to make a valid declaration. For the error estimation the Gaussian propagation of uncertainty[6] was used.

3 Theoretical Model

In the following a basic theoretical model will be presented. Mainly the model gives proportionalities and explains the changes of the characteristics' values during a packing process.

3.1 Potential Energy

It is stated that every packing wants to reach a state where it is as stable as possible. The less energy is stored in the packing the more stable it is. The packing is compacted by shaking it vertically with an amplitude a and a frequency f. Every particle in this packing has a potential energy E_{pot_p}. The position of the center of mass given by the y-coordinate h_p defines the value of E_{pot_p}. The potential energy decreases if h_p also decreases. The energy of every particle added is the potential energy of the whole packing, E_{pot}. That basically means if a packing is loosely packed the potential energy of it is higher than the energy of the same packing when it is densely packed.



$$h_{p_1} < h_{p_2} \Rightarrow E_{pot_{p_1}} < E_{pot_{p_2}}$$

Figure 5: Examples of h_p and E_{pot_p}

When an *RLP* is created the particles will not fall on the lowest possible energy level because the friction between them is stronger than the gravitational force $F_g = m \cdot g$. To overcome the friction energy has to be added to the packing: a packing process. The particles have to be lifted up so that they can fall down again, which gives them kinetic energy. The kinetic energy has to have a higher value than the energy which is needed to overcome the friction, otherwise the particles would have the same or even higher E_{pot_p} values as before.

3.1.1 Friction and Activation Energy

The minimum energy which is necessary to lift the particles as far up as a decrease of h_p requires is called the activation energy E_A. An important aspect concerning predictions for the required energy E_A is the friction between the particles. Our theory states that the friction coefficient f is proportional to E_A:

$$F_f = f \cdot F_g \tag{4}$$

When the packing is denser, which implies more contact area, more energy is required. The result of this relationship is a logarithmic increase of the density if the energy which is applied to the packing stays constant over the time.

3.1.2 Statistical Reasoning

Another reason for a logarithmic increase of the density during a packing process with a constant frequency and amplitude has a statical background. Even if E_A is theoretically high enough a particle has to have a gap into which it can fall so that it can achieve a lower value for h_p. Figure 3 illustrates this correlation: The free space another particle could take decreases and so does the probability that it is actually placed in a way that it could fall to a lower energy level by applying E_A.

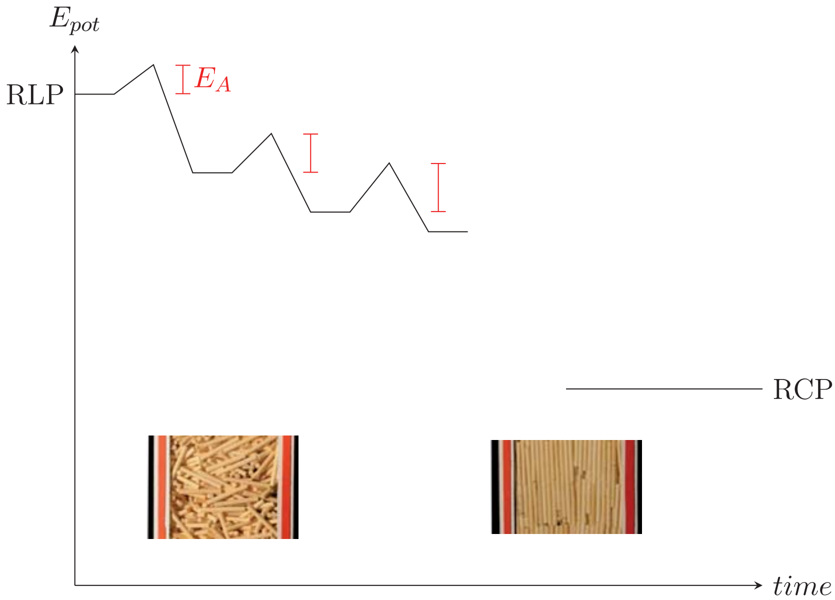


Figure 6: Evolution of potential energy inside the packing

3.2 Change of the Coordination Number

It is stated that a higher average coordination number implies a higher density [10]. Figure 7 visualizes this correlation. The first few measurements were taken from a packing of matches with a very low solid volume fraction below the average density value for a *RLP*. This was achieved by placing each one of the matches by hand into the box. Density values over 0.4 were created by compacting a *RLP*. With the measurement method presented in section 2.2.2 the average coordination number of the packing was determined. The plot shows a non-linear growth until the maximum of the coordination number is reached. Why there is a maximum is explained in the following.

3.2.1 Comparison with Crystal Structures

A packing can be seen as a crystal. The definition says that a crystal is a solid material whose constituents, such as atoms, molecules or ions, are arranged in a highly ordered microscopic structure, forming a crystal lattice that extends in all directions [2]. The term "highly ordered" implies that the crystal properties can be described by a unit cell. A unit cell represents the characteristic structure with its coordination number and free space. It can be considered as a packing of spheres where the free space describes the solid volume fraction of the unit cell. Sphere packings are already well studied [5]. Hereby the spheres considered are usually all of identical size in a three-dimensional Euclidean space [14]. The properties of such a crystal are similar to the properties of a packing: the coordination number of every component inside a crystal is the same whereas in a packing the distribution of this number for every particle is Gaussian[2]. Because of this Gaussian coordination number distribution the density of a packing consisting of non-spherical materials cannot be calculated. Figure 8 shows a few examples of crystal structures. Direct comparison of a sphere

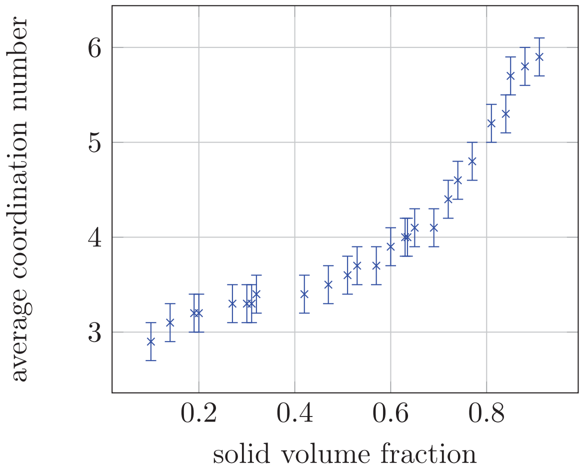


Figure 7: Average coordination number in a packing of matches

Unit cell	Coordination number	Space
Simple Cubic	6	0.52
Body-Centered Cubic	8	0.68
Face-Centered	12	0.74
Hexagonal Closest Packed	12	0.74

Figure 8: Crystal structures and their most important properties coordination number and free space

packing with well known properties with the work in this thesis, which is focused on non- spherical particles, is not possible. But the correlations between coordination number and the free space between the particles achieved by both types of study are the same [12].

4 Parameters of a Packing Process

4.1 Duration

The investigation of the parameter duration is the most trivial one. As it is explained in the theoretical model (section 3.1) adding energy to a packing results in the packing becoming denser. So the longer a packing is put under a compacting process the more energy is added and the solid volume fraction increases.

4.2 Direction

The most interesting question regarding the packing process is how it is performed. There are three basic methods: horizontal, vertical and rotational shaking (see figure 9). Shaking a box by hand would make the experiments unreproducible. That is why a self-built shaker was used. A plate was mounted on a speaker which was connected with a frequency generator and an amplifier. This construction allows an exact variation of the frequency and amplitude of the shaker. The method of shaking the packing vertically is easy to realize by simply putting the speaker with

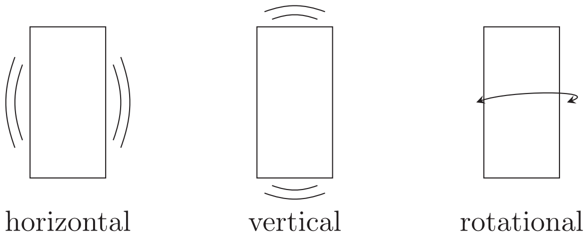


Figure 9: Three different methods of shaking a box

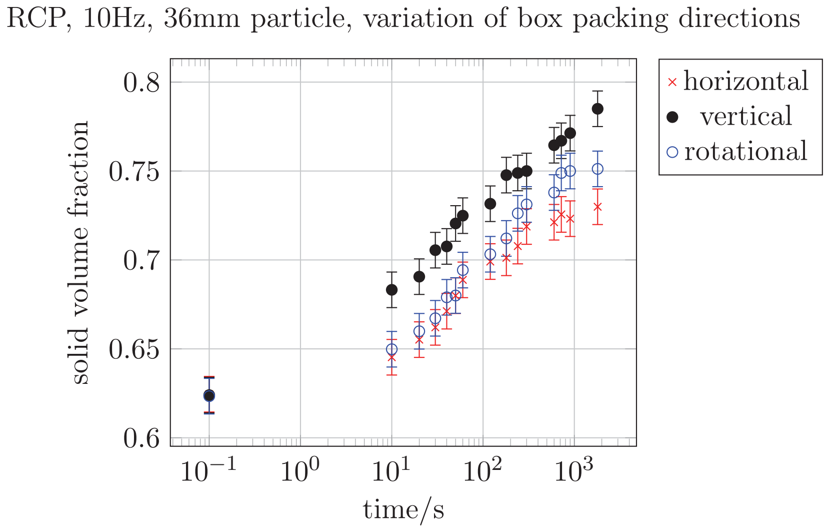


Figure 10: Investigation of the three different methods of compacting a packing effectively

the plate parallel to the ground. For a horizontal shaking the plate has to be mounted perpendicular to the speaker plane. An electric drill was modified to shake a packing by rotating it but due to technical failures this method was not investigated further.

In the series of experiments investigating the packing direction the vertical method worked the best. To explain why, the theoretical model has to be considered (see section 3.1). With the horizontal and rotational method the particles have to overcome more dynamic friction than with the vertical method.

4.3 Frequency

How well a packing is compacted is only dependent on the energy added to it. The higher the frequency is the less time the packing process takes.

4.4 Amplitude

A higher amplitude of a shaker implies a faster packing process due to the theoretical model (section 3.1). To verify the theory a series of experiments were made using the vertical packing method with the amplitudes 0.5cm, 1.0cm and 2.0cm. Figure 11 shows the results, which confirm the theoretical predictions. At the beginning

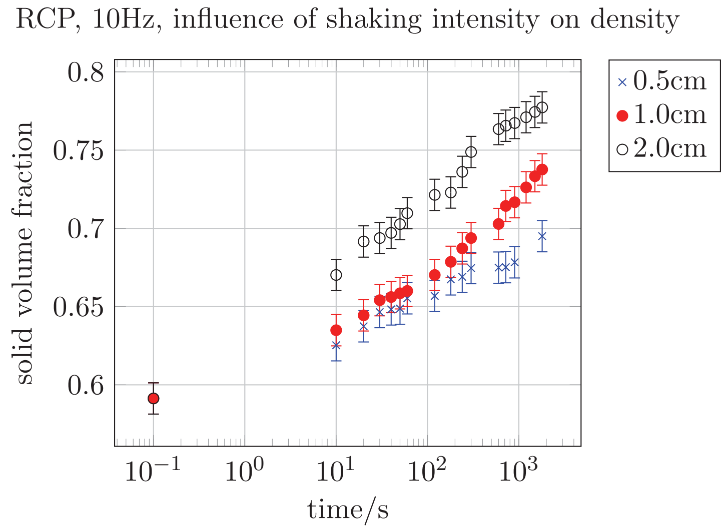


Figure 11: Investigation of different amplitudes

of the process until around 10^2 seconds the 0.5cm and the 1.0cm treatments do not differ much, but as the duration is extended one can see the solid volume fraction increases significantly for the 1.0cm experiment. The 2.0cm treatment shows a more effective packing process from the beginning compared to the experiments with a lower packing amplitude.

4.4.1 Minimal and Maximal Amplitude

There is the remaining question of whether limits exist for the amplitude. As already shown in section 3.1.1 there has to be a certain activation energy E_A to overcome the friction. This fact implies that there is minimum for the amplitude if a packing should be compacted. There is also a maximum. If a packing is shaken too intensely it causes the same effect than randomly filling a box would cause.

5 Box, Filling and Material Parameters

There is already some research performed which considers the relationship between filling height, box and particle dimensions [15].

$$\frac{H_{Cri}}{D} = 90.29 \cdot \left(\frac{d_v}{D}\right)^{1.41} \tag{5}$$

H_{Cri} stands for the so called critical filling height, D for the box diameter and d_v for the equivalent volume diameter of a particle.

5.1 The Meaning of the Critical Filling Height

The theory [15] behind equation 5 states that there has to be a certain relation between the filling height, box and particle geometry to determine the correct density value for the RLP for a certain kind of granular material. Figure 12 shows a theory plot: If only a very small amount of particles is in the box the measured value for the density is lower compared to the density in a box with a higher filling height.

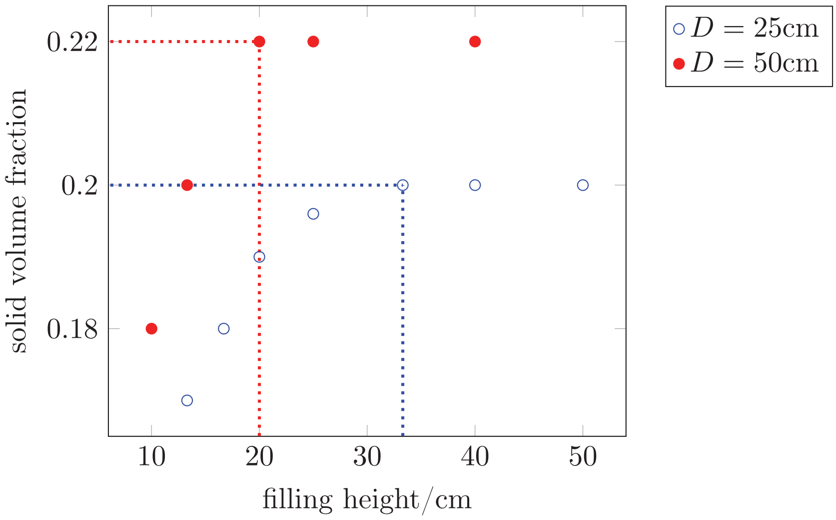


Figure 12: The effect of the critical filling height

This effect is known as the Wall Effect. After a certain filling height is reached the density stays constant and now the correct value for the *RLP* can be determined. Because the density difference is usually smaller then the measurement errors given by failures in determining the particle volume and the data analysis presented in section 2.2 we could not test this theory in our experiments.

5.2 Wall Effect during the Packing Process

Even though the Wall Effect cannot be observed in an *RLP* with conventional methods it is clearly visible in a packing process. Figure 13 shows our experimental setup: The same granular materials were used to fill different boxes. The graph shows that the theoretical calculated critical filling height is dependent on the box diameter. The bars represent the difference of H_{Cri} and the actual filling hight. Two experiments were performed with a filling height under the required height H_{Cri} (in the plot the red and the black bar). Therefore for these experiments the Wall Effect occurs theoretically in the *RLP*. The blue bar represents an experiment with a filling height far above H_{Cri}. The results are quite stunning: in the experiment where no Wall Effect occurs (blue) in figure 14 the density increases logarithmically as predicted in section 3.1.1. For a small difference of H_{Cri} and H (black) the same increase can be observed until at a certain point the density growth slowly stops before the packing is much faster packed than in the increase phase before. The same phenomenon is visible for a large $H_{Cri} - H$ difference (red). The length of the phase of a logarithmic density increase hardly differs from the smaller $H_{Cri} - H$ distinction experiment. But there is no real identifiable stop in the density growth, to the contrary the solid volume fraction suddenly extends with a major exponent than before until the packing reaches the state of an *RCP*.

5.3 Qualitative Explanation

We assume that the particles are distributed randomly. That means every combination of the two defining angles which tell how a particle is orientated exists equally. But a random distribution like this is only permitted if every orientation of the

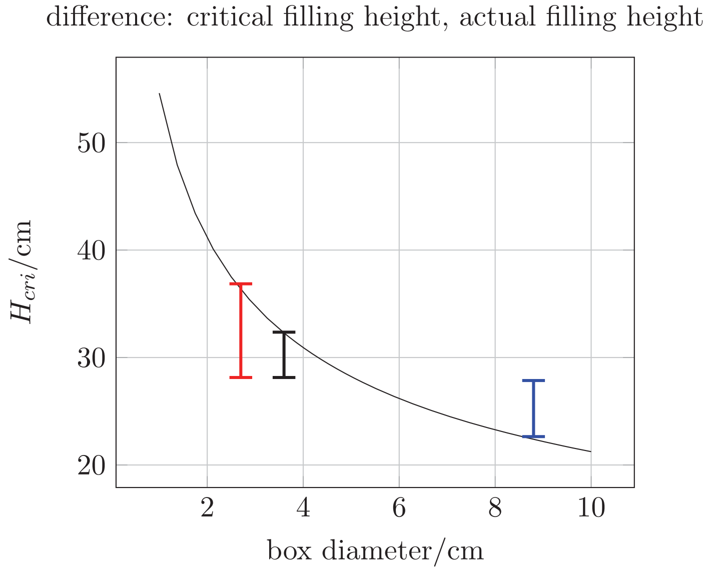


Figure 13: H_{Cri} and actual H of the same box

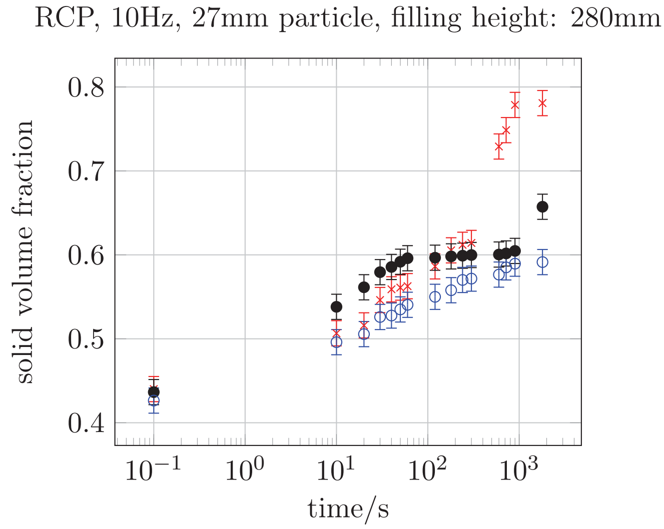


Figure 14: Wall Effect during a Packing Process

particles is possible by the given box geometry. It is not permitted if the particle dimensions are equal or greater than the box dimensions. If this is the case a particle is restricted in his orientation. Figure 15 shows the situation: A restriction ($D < d$) leads to a maximum orientation angle θ_{max}. To simplify the qualitative explanation we consider the box to be two dimensional. Another assumption is that the particle has a certain length d but no width which has to be taken into account for an exact calculation of θ_{max}:

$$\theta_{max} \approx \frac{\pi}{2} - \arccos\frac{D}{d} \tag{6}$$

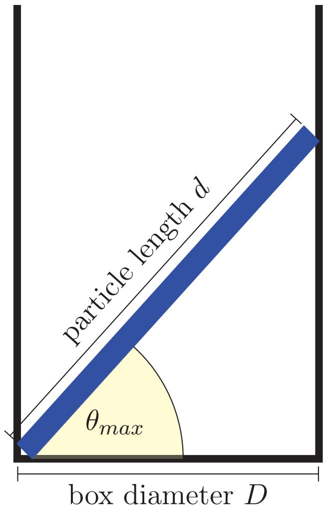


Figure 15: Geometry of a particle in a box

5.3.1 Influence of the Orientational Order

As one can see in figure 2 the particles in a densely packed packing are all ordered in the same direction because an orientational order like this implies a minimum of the void volume fraction. In every experiment the particles aligned themselves vertically. If a θ_{max} does not exist particles lying in a horizontal manner have to be lifted up 90 degrees which obviously takes more energy than arranging a particle which has a non-horizontal orientation. So θ_{max} is representing the highest value of the energy which is needed to align a particle inside the packing. The orientation angles in a two dimensional packing are distributed randomly between 0° and θ_{max}. Because of the restriction in the distribution the energy which is needed to pack the packing is lower in comparison to a box with the case $D \gg d$. Therefore a packing process takes less time. This effect also occurs not only if $D < d$ but also when the particle and the box dimensions are in the same order of magnitude as it can be seen in the experiment in figure 14. Those disorders in the orientational order decrease in proportion to the greater D is in comparison to d.

5.4 Filling Rate

Before one can start an investigation of an *RLP* a box has to be filled with particles. A justified assumption would be that the manner of filling has an influence on the packing. Putting the granules in the box one by one makes a broad range of different

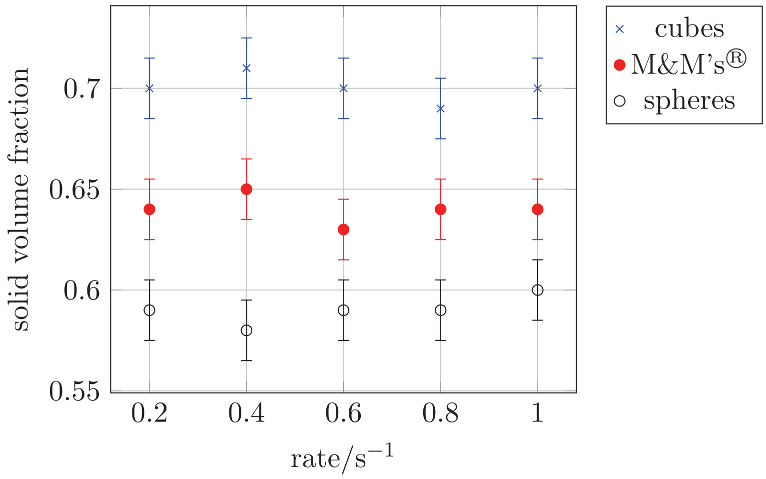


Figure 16: *RLP* after different filling rates

orientational orders possible which can be fully controlled by the individual filling the box. So our assumption is that we *pour* the granules in. The most important parameter here is the filling rate. Different materials were used to determine the influence of the rate. The box was filled in different experiments with cubes, M&Ms and spheres in rates of $0.2\text{s}^{-1} - 1\text{s}^{-1}$. A rate of 0.2s^{-1} means that the box was filled with particles at a rate that was five times slower than in an experiment that filled the box at a rate of 1s^{-1} ("everything was poured in at once"). After each try the density was measured. The plot 16 shows the experimental results: the solid volume fraction difference between the experiments is always within the measurement errors. This leads to the conclusion that either the difference is so small that it cannot be recognized with the methods presented before or the filling rate has no influence at all.

5.4.1 Mathematical Approach

As it was described in section 3.1 adding energy to a packing makes it denser. To give an explanation why the filling rate has no influence on the properties of a *RLP* a comparison between the two extreme cases is given: pouring in particle for particle (very low rate) and pouring in everything at once (very high rate). If n is the number of particles, m the mass of a single particle and h the height from where each particle is poured in the energy which was added to the packing when it is fully filled can be calculated in a simplified way:

$$E = \sum_{k=1}^{n} = m_k \cdot g \cdot h_k \tag{7}$$

Considering the fact that a packing consists always of particles of equal properties and the height stays constant for all falling particles the equation is now equivalent to the "everything at once" calculation:

$$E = n \cdot m \cdot g \cdot h \tag{8}$$

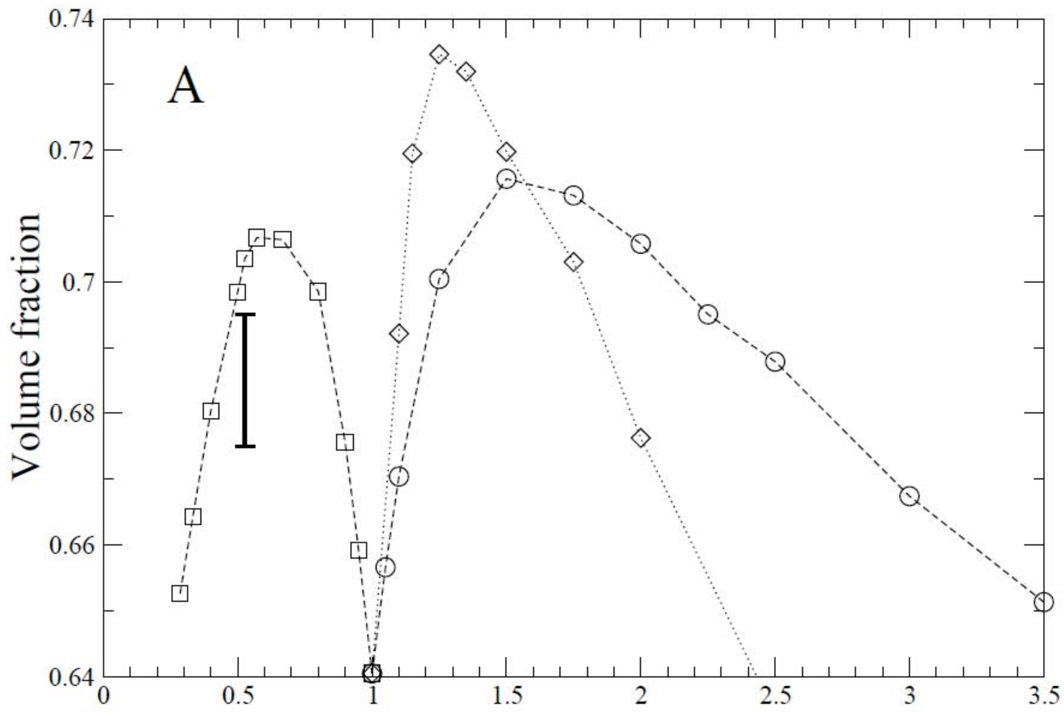


Figure 17: Influence of the aspect ratio on the *RLP*[4]

5.5 Aspect Ratio

The aspect ratio of a geometric shape is the ratio of its sizes in different dimensions. For three dimensional shapes such as the particles considered in this thesis the aspect ratio can be defined as the ratio of the longest side to the shortest side [11]. For example, speaking of ellipsoids such as M&M's®or Smarties®an aspect ratio of 1 represents the shape of a sphere and for cuboids such as matches a cube would have an aspect ratio of 1.

5.5.1 Influence on the *RLP*

The influence of the aspect ratio on the *RLP* is already well studied [4]. Figure 17 is an example for the aspect ratio - density relation: A local density minimum occurs if the aspect ratio equals 1. The more "stretched" a particle is, the higher is the intensity increase up to a maximum value of around 1.5. Then the solid volume fraction decreases again. A higher aspect ratio usually implies a bigger surface of a particle where friction forces can hold the packing together. This is the explanation why the density decreases with an increasing aspect ratio value from a certain value on. The local minimum for the value 1 is a special case and has been investigated by various studies[1], but was not investigated in this research project.

5.5.2 Influence on the Packing Process

For this dependency investigation cylindrical particles in the form of brochette spikes were used. The spikes were cut into different lengths to obtain packings of particles of the aspect ratio 6, 9 and 12. Those packings were put under a packing process. In figure 18 the results are presented: The packings start with a different density

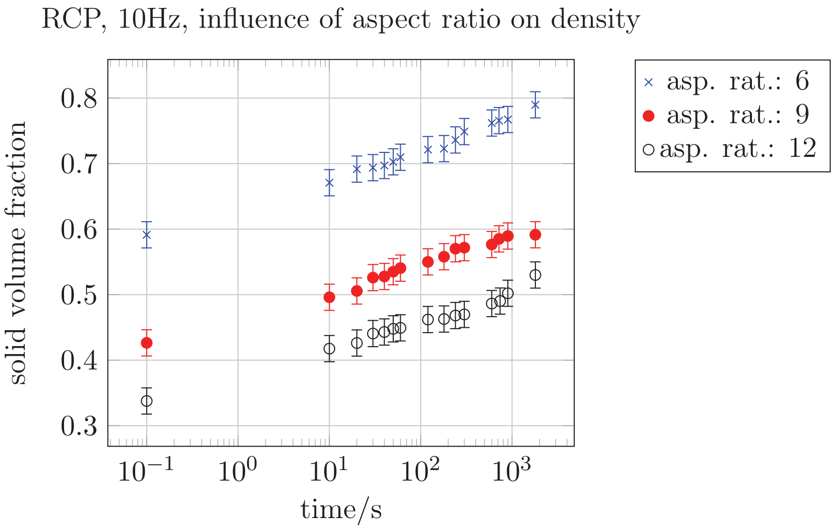


Figure 18: Influence of the aspect ratio

due to the aspect ratio value difference explained in section 5.5.1. Furthermore the particles are packed nearly with the same effectivity.

6 Conclusion

A packing can be well described by its coordination number, orientational order and density. The changes of these characteristics during a packing process are predictable to a certain extent if the box, particle and packing properties are known. There is already a comprehensive research done considering the different stadiums of packing regarding particle properties such as the characteristic shape. Therefore for every granular material which is used boundary values for the different packing conditions can be given.

The box properties do not have to be taken into account as long as the ratio of box and particle dimensions is great enough. If this is not the case the so called wall effect occurs which has an influence on the orientational order. The relation between the orientational order and the density is the proportionality of the orientational angle distribution to the solid volume fraction. If a packing consists of very well ordered components it will be denser than the same packing with an equal orientational angle distribution.

There is also a critical filling height for each packing. If the box is filled more than H_{Cri} no remarkable effect appears during a packing process. But if this critical height is undercut irregular density changes occur.

An investigation of the packing process parameters was performed to better define the solution of the century old Packing Problem: How should we arrange objects to pack them as tightly as possible, making best use of all the available space? A first arrangement of objects is obtained by the actual creation of a packing, the filling. The research in this paper concluded that there is no significant influence of the filling rate on the random loose packing except the case placing the objects in the box by hand, which was not included in this thesis.

A theoretical model is presented for what is actually happening during a process of compacting granular materials and how one can influence this process. The aim is a preferably effective transformation from a random loose packing to a closely packed one. To achieve this goal the optimal method has to be found. It was concluded that using a shaker vertically provides the best results. Finding the optimal amplitude and frequency is also an important aspect. In particular, the boundary values for the amplitude have to be considered because the theoretical model predicts the existence of a minimum of energy which has to be added to the packing so the friction and gravitation force can be overcome. For every experiment precise error expectations could be given even though the high errors resulting from the limited accuracy of the experimental method restricted a good validation of theories taken from literature.

Using three dimensional computer simulations for all parameter investigations considering the Packing Problem would lead to an immense improvement of precision in the actual experiments and in the data analysis. Despite creation of an analysis script for the density calculation, no help from computers was used which demonstrates that approaching the Packing Problem in a scientific way is easily possible.

Remarks

The topic of this thesis was adapted from a problem posed in the International Young Physicists' Tournament (IYPT) 2015:

The fraction of space occupied by granular particles depends on their shape. Pour non-spherical particles such as rice, matches, or M&M's candies into a box. How do characteristics like coordination number, orientational order, or the random close packing fraction depend on the relevant parameters?[1]

As a member of the German national team for the IYPT 2015 in Thailand I was was given the opportunity to discuss the Packing Problem with highly qualified people from all over the world including other students, teachers and professors. I would like to thank everybody who supported me during my research into this problem especially staff from the Schülerforschungszentrum Ulm for providing laboratory equipment and scientific help.

List of Figures

Declaration of Authorship

I hereby certify that this thesis has been com posed by me and is based on my own work, unless stated otherwise. No other person's work has been used without due acknowledgement in this thesis. All references and verbatim extracts have been quoted, and all sources of information, including graphs and data sets, have been specifically acknowledged.

[1]http://iypt.org/images/8/87/problems2015.pdf

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