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A novel approach to predicting the behavior of arbitrary particulate mixtures under vibration

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Abstract

A novel, digitally based geometrical packing algorithm, called DigiPac, is used in an investigation into the segregation of non-spherical particles, due to vibration or shaking. Comparison between simulations and experiments shows a consistent, albeit qualitative, correlation, supporting the hypothesis that segregation can be explained from a geometrical instead of mechanistic point of view, in terms of relative mobility between particles of different shapes and sizes. Thus, although the geometrical packing algorithm cannot be used to follow the dynamics of a segregation process, it provides a software tool for quick trend finding as to if and how likely segregation is to occur for any given mixture of arbitrary shapes. Such a tool is useful for process design and optimization of particulate solids.

Keywords: segregation, non-spherical particles, packing, vibration.

1. Introduction

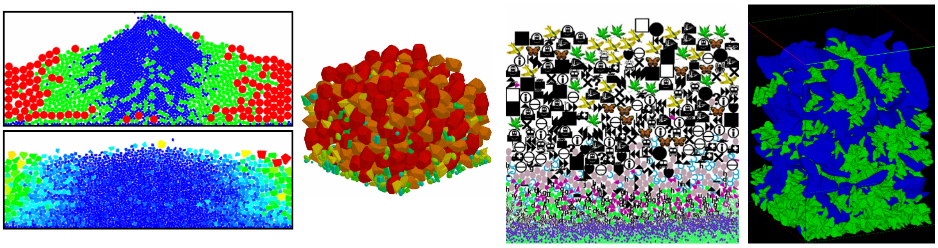
Whilst considerable effort has been reported on computational approaches to describe packing and segregation of populations composed of uniform or size polydisperse particles of regular geometric shape (mostly spheres), simulation of the behavior of systems that have arbitrary shapes and sizes have not been considered. The development and application of such a capability is presented in this paper. Particle segregation is the tendency for some components of a mixture to move from one zone to another and to be concentrated there based on their physical and geometrical attributes. Segregation is often involuntary and unavoidable, resulting from handling particulate mixtures. At present, there is no single consensus on segregation and what the main driving forces behind it are. Some researchers [1] attribute it to the fact that the various forces that act on the individual components of a particulate mixture may cause them to move in different directions, or to different positions in a bulk, due to their differing characteristics. Commonly, the most important of these characteristics is size, although shape, density, surface roughness, resilience, electrostatic properties and moisture can all play a role [2].

The theory proposed by this paper is that mechanical interactions are the driving force that cause the relative motion between particles, yet it is the geometrical factors, namely size and shape, that ultimately determine if segregation occurs. This investigation aims to fill the gap left by many past studies where the significance of the geometry or shape of particles has been recognized but largely ignored, mainly due to limitations of other computer models to simulate complex shaped particles and their movements.

2. Model Description

The basic ethos of the digital packing algorithm, known as DigiPac [3], is of treating each particle as a coherent collection of pixels rather than a geometric object. Compared to conventional vector-based approaches, this allows particles of arbitrary shapes to be represented and manipulated in a much more straightforward and computationally efficient manner, in a simulation environment. For example, collision and overlap detection is usually the hardest to code and most time-consuming to run for vector based simulation software; in DigiPac, this is a simple matter of checking double occupancy in the regular lattice grid which hosts the digitized particles, container or packing space.

In the original version of DigiPac used for this investigation, particle interaction forces are not explicitly considered. Particles essentially undergo a preferential random movement. At each step, a random direction out of all possible directions (6 in 2D and 26 in 3D) is first selected; if the move contains an upward direction (e.g., north in a move to the north-west in 2D), the upward movement is only effected with a so-called rebounding probability, thus giving the otherwise complete random motion a downward preference, to simulate the effect of gravity. This rebounding probability (RP) can also be used to mimic the effect of vertical vibration. For example, RP = 0 means no vertical vibration, since no upward movement is ever allowed and particles can only move laterally and/or downward. RP = 1, on the other hand, corresponds to a most vigorous vertical vibration, where particles have equal probability of moving up or down, and are therefore forever suspended. It has been observed that when packing a mixture of different particle shapes and/or sizes, segregation tends to take place, particularly if vibration is turned on and/or particles are dropped from a narrow orifice. Fig.1a shows two examples: one in 2D showing the so-called Christmas tree effect; the other a pile of crystals in 3D.



(a) (b)

Fig.1 Examples of segregation due to (a) vibration and (b) shaking.

Shaking can be simulated by repeating the process whereby the packed bed is lifted *en mass* and particles are then allowed to resettle. This procedure has been used before by Jullien et al [4] to simulate segregation of spheres. With DigiPac, the simulation can easily be extended to include non-spherical and complex shapes, as demonstrated in Fig.1b.

DigiPac was not originally designed with simulating segregation in mind, yet despite its simplicity and lack of explicit consideration of physical interaction forces (other than gravity and the non-overlap constraint), segregation has been observed in most packing simulations that involve different sizes/shapes. This has prompted us to postulate that segregation is predominantly a geometrical effect. In other words, whether or not segregation is to occur in a given mixture, or how quickly segregation takes place in one mixture relative to another, is determined by geometrical factors such as size and shape (which includes both the overall form and detailed surface texture or roughness). For a mixture of different sized/shaped particles, all that is needed for segregation is relative motion – it does not matter how the relative motion is achieved. Inter-particle, and externally applied, forces are merely means to promote or hinder relative motion; they are themselves not the root cause for segregation. If this is true, then a geometrical packing model such as DigiPac is adequate for predicting if segregation is to happen and the *relative* rate at which mixtures of different compositions segregate under vibration or shaking. A mixture such as a free-flowing powder that is easy to segregate under vibration/shaking is usually also prone to segregation under other handling procedures. Therefore, the simulation results can provide a general indicator of 'segregatibility'. In this investigation, the number of shakes required for segregation to occur is used as the indicator.

3. Experiments

To test the hypothesis, a pseudo 2D transparent box with adjustable gap width was constructed. A tap density tester (Copley JV 2000) was used to provide the vibration. For 3D tests, a cylindrical container and a sieve shaker were used.

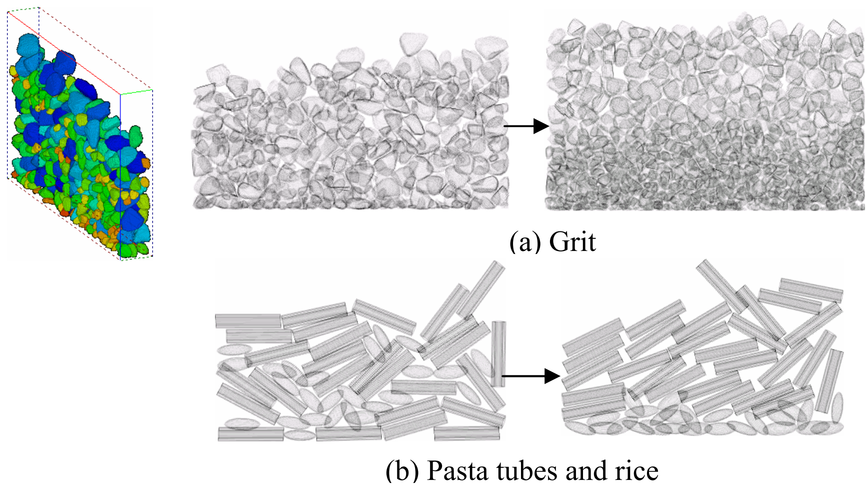


Fig.2 Examples of tested mixtures, from mixed to segregated states.

	Exp	Sim
grit only	6700	205
grit & pasta	8850	304
grit & rice	7900	229
grit & fine sand	5400	193
pasta & fine sand	6800	162
rice & fine sand	7500	211
pasta & rice	9050	287

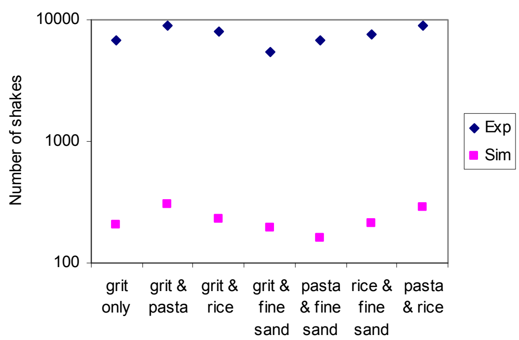


Fig.3 Comparison between experimental and simulation results (pseudo 2D).

4. Comparison Between Simulations and Experiments

Mixtures of different size and shaped objects were tested in the pseudo 2D setup. Some examples are given in Fig.2, and Fig.3 shows the results. These correspond with segregation by vibration. Although the number of shakes required for segregation to take place in the experiments is more than an order of magnitude higher than from the simulations in each case, the trend is consistent and almost the same.

In 3D tests – segregation by shaking – the same similarity has again been observed. Fig.4 shows two examples, where two types (i.e., spiral shaped and shell shaped) of whole and broken pasta pieces were used. X-ray microtomography was used to scan the pasta pieces for use in the simulations. Whole pasta pieces were randomly and digitally chopped in the simulations to have the same mean size as the broken pieces in the experiments. Tests at different size ratios show that although the experimentally observed number of shakes is higher than the simulated, the plots are more or less parallel in each case.

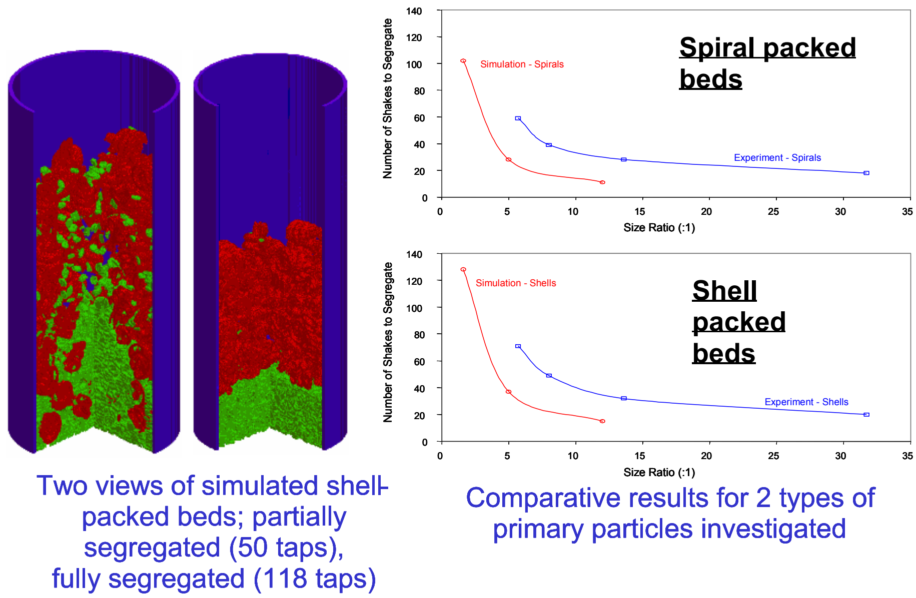


Fig.4 Comparison between experimental and simulation results.

5. Conclusions and Future Work

Comparisons between simulations and experiments in both pseudo 2D and full 3D have shown that DigiPac – a simple geometrical and stochastic packing algorithm – is able to predict qualitatively correctly the trend for segregation in different mixtures of complex shaped particles, thus supporting the hypothesis that it is the geometrical factors that determine if and how likely segregation is to occur.

Further tests are being performed, and to be extended to powders. For powders, a virtual setup with periodical boundary conditions is to be used in the simulations. This allows a small number of particles to be used to simulate the bulk behavior, keeping the computational burden at a manageable level.

It is believed that mobility is closely linked with the coordination numbers of different shapes. Future work will focus on relating the number of shakes (the segregatibility index) with geometrical factors such as the mean coordination number and proportion of each shape in a mixture. If such a correlation can be established, then predicting relative segreagtibility becomes even simpler and faster, since working out the mean coordination number of each shape in a given mixture requires only one packing simulation involving a minimal number of particles. Experimentally, the mean coordination number can also be obtained from X-ray tomography imaging of the mixture. A simple and fast procedure like this can provide a design tool for product formulators.

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