Geometric aspects of particle segregation

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Size segregation is a natural occurrence both in everyday life and in industrial processes. Understanding and research of the phenomenon has overwhelmingly been from a mechanistic point of view. This paper demonstrates through simulations that segregation can also be explained and trends predicted geometrically. The algorithm used in this study contains three simple elements: random walks combined with a rebounding probability to encourage particles to settle, plus the nonoverlap constraint. It is implemented digitally in a regular lattice grid, to make it easy to deal with arbitrary shapes. It does not explicitly consider any particle interaction forces, and it does not include any rules specifically designed to promote or suppress segregation. Yet particle movement, which occurs within a digitized cubic grid, leads to shaking-induced segregation comparable to that observed in physical tests. The paper details the comparison of shaking-induced particle segregation between a series of computer based simulations and those of physical experiments undertaken in the laboratory. A range of mixtures, comprising nonspherical, arbitrary shaped/sized particles are investigated, having been packed into pseudo-two-dimensional containers. The simulation results suggest that segregation can be adequately explained, from a geometrical point of view, as a result of the relative motion between particles of different sizes and shapes. The geometrical algorithm thus provides a fast and qualitative prediction as to how likely segregation is to occur for any given mixture of arbitrary shapes.

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I. INTRODUCTION

Particle segregation is a naturally occurring and frequently observed phenomenon where particles of different characteristics separate when a particulate system is subjected to some form of agitation such as flow, vibration, shaking, rotation, or stirring. A number of theories [1–3] and computer models [4–12] have been proposed in an attempt to explain it, but to date a consensus and generally applicable explanation remains elusive. Some researchers [13] attribute segregation 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 the bulk, due to their differing characteristics. The most widely acknowledged characteristic is relative particle size, although other features suggested to play a role include shape, density, surface roughness, resilience, electrostatic properties, and moisture [14,15], as can the external forces acting upon a system. Subsequently, the majority of the fundamental mechanisms, which can result in segregation were collated by [16], who also demonstrated that process conditions play a major role in determining which mechanisms will play a dominant role in any given situation. It is apparent that many studies have tended to concentrate on either physical experiments or computer-based simulations [7,17], only rarely combining the two [18].

While the majority of these do acknowledge that relative particle size (more so than shape) has a significant influence on the pattern of segregation, the majority choose to focus on the effects of mechanical or dynamic aspects of the process as the primary factor responsible for driving segregation [19,20]. In addition, considerable effort has been reported on descriptions of packing and segregation of different populations (composed of both uniform and size polydisperse particles) of regular geometric shape (mostly spheres), despite the fact that real particles are rarely perfectly spherical. There are at least two possible reasons for this: a) theoretically, modeling of nonspherical particles and their behavior has been difficult; b) experimentally, particle shape introduces an extra complexity in data analysis which does not help to elucidate the root cause of the so-called "size" segregation. As a consequence, simulations of the behavior of systems that are comprised of arbitrary shapes and sizes have not been considered, particularly in terms of segregation.

In this work, a series of computer-based experiments are presented with attention focused on the segregation of nonsticky arbitrary shaped/sized objects, with results compared against experimental data as a means of qualitative validation. Computational investigation is undertaken using a digital-based geometrical packing algorithm called DigiPac [21]. The geometrical packing model used was not originally designed with the intention of simulating segregation, yet despite its simplicity and lack of explicit consideration of physical interaction forces (other than gravity and the nonoverlap constraint), segregation has been observed in most packing simulations that involve different sizes/shapes of particles. In this paper, we examine segregation from a geometrical instead of mechanistic point of view. Our proposition is that, whether or not segregation will occur in a dry granular mixture, or how quickly one component separates from another in a given mixture relative to other mixtures, is primarily determined by geometrical factors as a result of relative motion or, more precisely, mobility between particles with different geometric properties, most often size and/or shape (which includes both the overall form and detailed surface texture or roughness), regardless of the exact physi-

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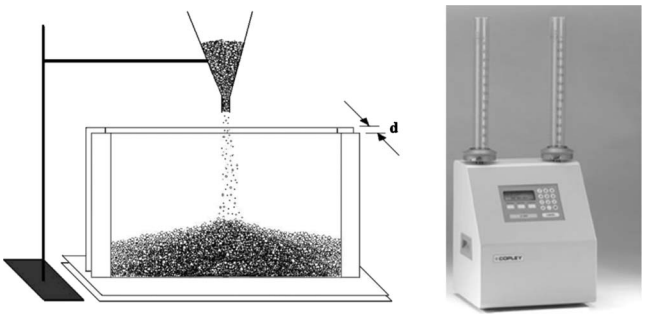

FIG. 1. (a) Modified Hele-Shaw cell used for investigation of arbitrary particles, showing adopted material loading procedure; (b) Copley JV2000 tap density tester.

cal or mechanical causes of the relative motions. These geometrically-based simulations are much faster than discrete element method (DEM) simulations for non-spherical particles. Even though the predictions are somewhat qualitative, for some applications, it provides a practical, cost-effective, and fit-for-purpose alternative to physical tests or DEM simulations.

II. METHODOLOGY—EXPERIMENT

The reported experiments were designed and performed by the authors. The experimental setup [Fig. 1(a)] utilized a self-constructed modified Hele-Shaw cell [22], which consists of two vertical Plexiglas sheets, 4 mm thick of area, 200 mm high by 300 mm long, mounted parallel to each other on a horizontal base plate. The front sheet was permanently fixed to the base plate, while the second was secured to the base by means of two aluminum "*L*" brackets in the lower corners, which allowed for position adjustment. By employing spacers that extend the full height of the vertical sheets (so that both ends remain closed) the separation distance, d, between the plates could be varied from 4 to 24 mm. The modified Hele-Shaw cell is attached to a tap density shaker.

The model of equipment used in obtaining the experimental results was a Copely JV2000 Tap Density meter [Fig. 1(b)]. Although not designed with such use in mind, the equipment is easily amenable to such uses, and proved to be effective as a shaking device for use in this investigation. The equipment was used to vibrate, vertically, the above described container with sinusoidal vibration amplitude, A, of 2.99 mm and a frequency, ν, of 250 Hz. On the front view of the equipment is a control panel and LC display to set the appropriate parameters and monitor the progress of the test.

The particles used in the investigation were arbitrary shaped, and classified into four key groups: crushed limestone grit (CLG) (Fig. 2), fine grain sand (FGS) (Fig. 3, and pasta tubes and rice grains. A total of seven mixture types were investigated in terms of comparative segregatability, six of which were binary mixtures and the remaining mixture consisted of crushed limestone grit only, which had a relatively wide particle size distribution. Each of the binary component mixtures were created on a 50:50 packed volume basis and were thoroughly mixed to ensure mixture uniformity prior to loading into the hopper used to charge the

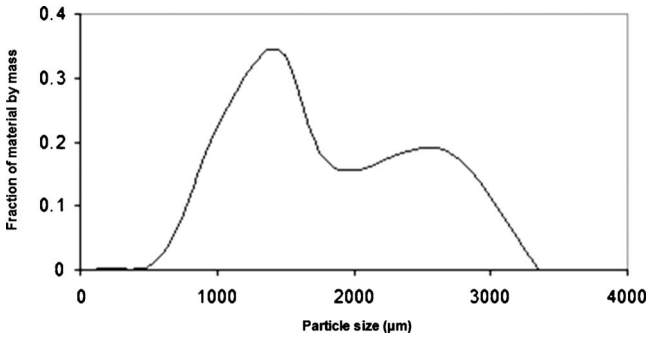

FIG. 2. Particle size distribution of crushed limestone grit.

modified cell [Fig. 1(a)]. By varying the height and lateral location of the hopper and rate of particle introduction, it was possible to effectively control particle addition and to transfer the hopper contents into the cell while minimizing any unwanted segregation (i.e., in the absence of bed vibration). When the complete mixtures had been transferred into the cell, the equipment was turned on, the bed repeatedly tapped and segregation was allowed to run its course, with visual observations made. When it was determined that segregation was complete, using a segregation index of 0.9, meaning 90% by volume of one component was in the upper half of the bed and 90% of the remaining component was in the lower bed half, the equipment was stopped and the total number of taps recorded. Additionally, each mixture was repacked and tapped a total of four times to ensure reproducible results.

III. METHODOLOGY—SIMULATION

The simulation model used in this study is the original and simplest version of DigiPac [21]. To distinguish it from later and more sophisticated versions, it is also referred to as DigiRWP—digitally implemented random walks based packing algorithm. In the context of this work, it can be described as a geometrical packing model that contains three basic elements. The first element is that particles undergo fixed-length random walks. Random walks have been used to simulate fractal aggregate formation for decades [23,24]. At an individual particle level, it is the simplest way to simulate diffusive random motions. In the context of particle packing, it is chosen for its simplicity and effectiveness, rather than

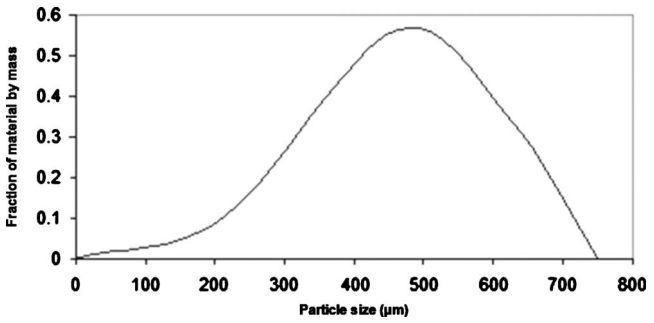

FIG. 3. Particle size distribution of fine grain (builder's) sand.

efficiency. The diffusive motion allows particles to effectively explore all available packing space without relying on particle-particle and particle-wall interaction forces to guide particles into obscure gaps or around obstacles of complex geometries. Software implementation of this is relatively easy and straightforward.

With random walks alone, particles would suspend in the packing space, but would not easily form a packed structure. To settle, particles must have their movements in the opposite direction of gravity somewhat restricted. To this end, a rebounding probability is used, which constitutes the second basic element of the packing algorithm. If the rebounding probability is set to 1, particles are free to move up and down with equal probability. The result is a suspended or fluidized state. If it is set to zero, no upward movement is allowed; and particles can only move sideways or downwards. In between, particles are allowed to move upwards from time to time, depending on the value of the rebounding probability. In a normal packing simulation setup, the probability is set between 0.1 and 0.5, to encourage particles to settle quickly while still have the ability to overcome local obstacles. For example, a particle dropped onto a relatively small trough will have a chance to move out in search of a tighter fit elsewhere if the rebounding probability is nonzero; but will be trapped there to form a less compact packing structure if the probability is zero. The two algorithmatic elements combined lead to a directional diffusive motion of the particles.

The third element is the nonoverlap constraint. Thus, if a random walk leads an object to overlap with another or the container wall, the trial move is discarded and the moving object is returned to its original position/orientation. A nonzero rebounding probability, which allows particles to move upwards occasionally, also gives particles a better chance to successfully tumble, i.e., rotate without resulting in overlaps.

Incidentally, for surface particles at least, a nonzero rebounding probability also creates a scenario similar to the effect of vibration. If one plays back a sequence of the simulated packing process, with a nonzero rebounding probability, particles at the top of the packed bed appear to be "boiling" over, i.e., moving and tumbling up and down violently. The same phenomenon is observed in practice if a bed is mechanically vibrated [25]. Particles embedded inside the bed are less affected, because of the nonoverlap constraint and lack of manoeuvring space. It is a known fact that vibration promotes segregation during the packing process, particularly if the particles are poured through a narrow orifice to form a heap. This has been observed in various packing simulations performed using DigiRWP, too many times for it to be regarded as a pure coincidence, and prompted us to consider segregation from a geometrical point of view.

Implementation details of the algorithm are fully described in [21] and will not be labored here. Suffice it to say, the fact that the algorithm is implemented digitally in a regular lattice grid makes it relatively easy to deal with arbitrary shapes; but digitization itself is not a contributing factor for segregation to occur in the simulations. The advantages of adopting a digital approach include the following. It makes no difference to software coding and simulation speed what shapes are involves in the simulations. Collision/overlap detection becomes a simple matter of checking if the same lattice site is being or about to be occupied by two particles, regardless of the complexity of their shapes.

In order to compare with results from controlled laboratory-scale experiments, a simulated shaking process is implemented, in the same way as described by Jullien *et al.* [7] for segregation of spheres. In essence, a bed is lifted up *en mass*, by a user-defined amount, at user-defined intervals then particles are allowed to resettle according to the DigiRWP algorithm. The process is repeated as many times as necessary, and stopped when 90% segregation is reached. Thus, in a sense, the current work is an extension of [7] to nonspherical particles. However, instead of a ballistic algorithm as used in [7], our approach is digital and this is a key that enables arbitrary shapes to be handled with relative ease.

The relative particle-particle and particle-container dimensions used in all the DigiRWP simulations were in direct proportion with those of the experimental investigations reported. A suitable size resolution (in pixels) was selected for the particles and receptacle in an attempt to obtain a good balance between limiting the degree of digital error while at the same time maintaining a reasonable simulation timeframe. As a general rule, the larger the digital container and particle sizes, the lower the difference in error from actual particles in terms of shape and roughness—the pixels used to build individual particles have close-up appearance of "staircases" as opposed to smooth edges. It therefore follows that the more pixels used to represent a digitized particle, the less intrusive these staircases would be, allowing a closer representation of the real particle. The downside to this, however, is that in DigiRWP the computational cost depends on the area or volume of the particle, regardless of the shape. Therefore, the greater the number of pixels used to construct a digital container (and the proportional particle sizes in order to maintain the aspect ratio of the experimental beds), the slower a simulation would run.

All of the simulations reported were started by generating the particles with random orientations, uniformly distributed in a box above the container and by allowing them to free fall, including fast, random axis rotation, into the receptacle. The simulation conditions, in terms of particle addition method and rate, intensity and the amplitude of shaking, were chosen so to quantitatively match those of the reported experimental results. When satisfied that each individual packing matrix was randomly and largely uniformly distributed throughout, the container was "tapped" as in the experiments, with vertical amplitude proportionally equal to that of the real beds.

IV. RESULTS AND DISCUSSION

Mixtures consisting of different size and shaped material were tested in the pseudo-2D setup described in Sec. II. The comparative results for the number of taps needed to separate different mixture types, and between corresponding experimental and simulated mixtures, are given later in Fig. 4. Although the number of taps required for segregation to take place in the experiments is more than an order of magnitude higher than for the simulations in each case, the trend is seen to be both qualitatively consistent and correlative. It should

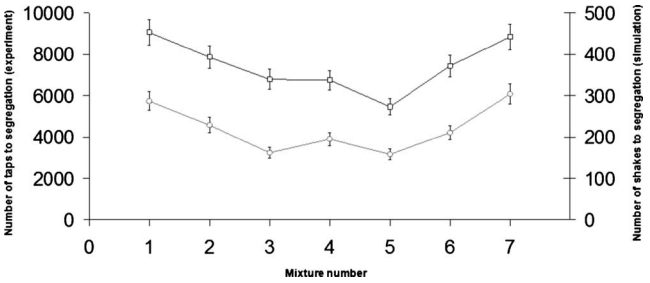

FIG. 4. Number of taps required to segregate the respective non-spherical mixtures presented in Table I. (Experiment—square; Simulation—circle).

be stressed that DigiRWP is a Monte Carlo (MC) type of simulation, MC cycles do not have a one-to-one correspondence with time step (or real time), therefore, it is *not* expected for the simulated and experimental results to agree quantitatively. It is the trend that matters.

A. Material types used

Sample 1: CLG.

Sample 2: Pasta tubes.

Tube diameter=3.1 mm, 0.7 mm central hole. Particles can be categorized in to two main groups:

(1) long, with slight curve; average length=26.3 mm, mean curvature=5^0;

(2) short, with great curve; average length=18.7 mm, mean curvature=8^0.

Sample 3: FGS.

Sample 4: Rice grains.

Grain diameter=1.4 mm. Approximately 7 mm in length.

Size distributions of the CLG and FGS were measured using sieve analysis, whereby the samples were vibrated for five minutes each, following which the different size fractions were weighed and presented.

B. Segregation results of the nonspherical mixtures investigated

For every mixture sample reported, the binary component mixtures were initially well distributed within the hopper before they were introduced into the container. Experimental samples were mixed in equal packed volumes, with a final packing height of approximately 100 mm and an internal container width of 145 mm. As we were mainly interested in what takes place along the length of the container rather than within the bulk of the bed, a container depth of 4 mm was used, enough for only one large particle in bed thickness, thus, providing a pseudo-two-dimensional (2D) arrangement, whereby the majority of relative particle movement could be observed from the front of the container.

In the reported results, beds were created using two methods:

Method 1: (pasta/grit, grit/sand, grit only) by introducing mixed particles from the hopper and slowly and periodically changing its lateral position from one end of the bed to the other numerous times until all the contents were *in situ*. During the simulation, the container was filled by allowing the particles to randomly "rain down" at a slow addition rate in order to recreate the method used to fill the container in the experimental runs, by moving the hopper from side to side, ensuring an even fill.

Method 2: (rice/sand, pasta/sand) The bed was created as a heap by keeping the lateral position of the hopper static and using the point source method for the simulations. Particles were present in approximately equal volumes, with the mixture thoroughly mixed before charging into the container. The heap was constructed by layers of particles, fed from overhead and flowing from the center to the edge of the heap. The individual layers were sheared because of a velocity gradient across each layer, causing smaller particles to collect closest to the filling point of the heap. The whole experimental procedure was repeated a minimum of three times, as for every bed investigated. In the simulation, the mixture was introduced using the hopper method with a reduced orifice size.

Small scale segregation is seen in local areas of the bed in addition to the bulk of the bed prior to any tapping occurring (caused by the unavoidable relative movement of particles during charging of the container). Figures 5–7 compare experimental and simulation results for five of the seven bed types investigated, corresponding to the number of taps given in Fig. 4.

C. Discussion

First of all, it is worth considering in some detail how the three basic model elements affect simulated results and what segregation mechanism can be revealed. It is helpful to repeat what the three elements are small fixed-length random walks, nonoverlap constraint, and a rebounding probability used to limited particle movement in certain directions.

Does the rebounding probability play an important role? The answer is not for shaking induced segregation. As has been mentioned earlier, use of the rebounding probability incidentally produces a vibration effect. However, as the simulations reported here use simulated shaking, by lifting the whole bed *en mass* periodically for resettling, this vibration effect is relatively small compared to the effect of shaking and therefore may be neglected. It is however necessary for creating a packed structure as it encourages particles to settle quickly.

What about the fixed-length random walks and nonoverlap constraint? The fixed length is defined by the size of a lattice grid in a DigiRWP simulation. (Note that a diagonal move can be regarded, and is implemented in DigiRWP, as a series of one grid cell orthogonal moves.) The reason for allowing particles to only move by one grid cell at a time was originally to avoid complications: a larger length can create a physically impossible situation, such as a particle going through another solid particle or jumping into a closed interior hole of another particle, which would require extra code and runtime to detect and prevent. The fixed length applies to particles of all sizes and shapes in the simulation. Thus, in unhindered settling, with zero rebounding probability, particles starting at the same height would reach the bottom at the same time, regardless of their size and shape, as if

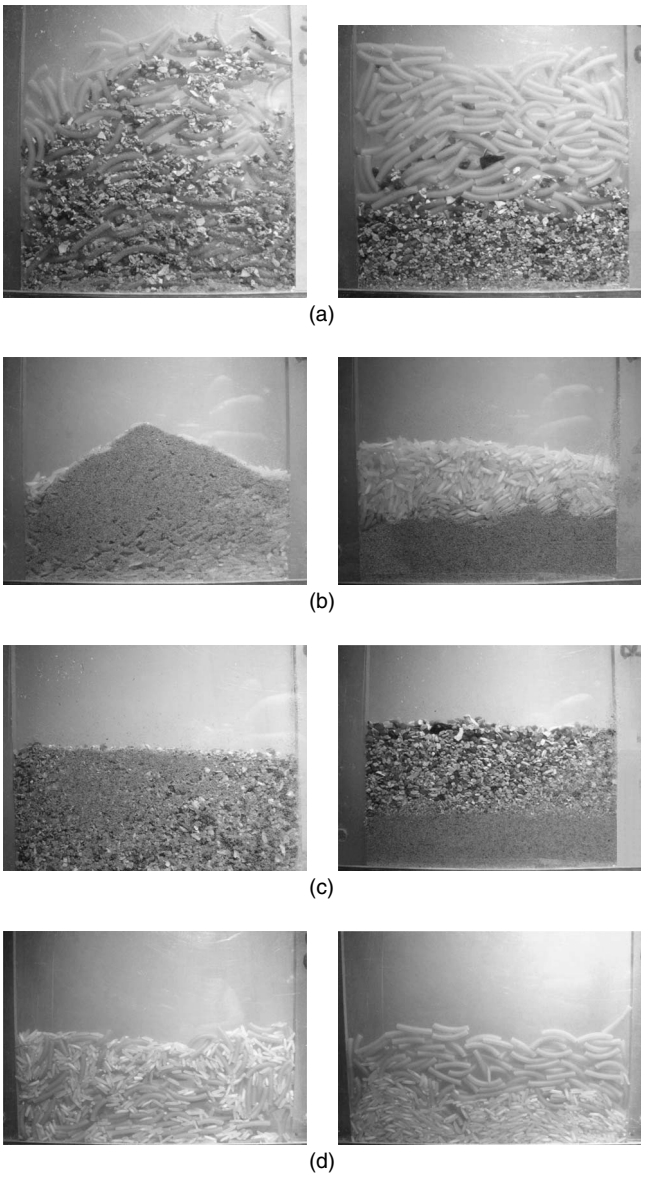

FIG. 5. Experimental results of mixed (left-hand column) and segregated (right-hand column) beds corresponding to number of taps shown in Fig. 4. (a) Pasta/CLG, (b) Rice/FGS, (c) CLG/FGS, and (d) Pasta/Rice.

they were traveling through vacuum under gravity. On the other hand, the fixed length creates a tendency for large particles to move a small distance relative to their size than small particles. In other words, small particles appear to be more energetic than large ones. This is generally the case in reality for packed particles, but for a different reason. In reality, how much a particle moves during a given time period is determined by interparticle and external forces according to Newton's law. In DigiRWP, this situation is effected by the nonoverlap constraint in conjunction with particle mobility. So, in the simulated world, fixed-length random walks, like physical forces, are only a means to create relative movements.

Mobility in this context means the average number of collisions during a given period of time or number of simulation steps. It depends on particle size *and* shape. A large particle surrounded by small particles would be difficult to move, because a move in any direction may generate overlaps. A small particle, given the same manoeuvring space, is comparatively more likely to succeed because it has fewer potential collisions. For two particles of different shapes, there is no such thing as "the same size." They may have equal equivalent size by volume or surface/projection area, but are unequal in other respects. This inequality is the reason why they have different mobility. There are examples where particles having equal equivalent volume size segregate under shaking [18]. DigiRWP created comparable segregations [26]. Therefore, although primarily designed to be a packing algorithm, DigiRWP can simulate the root cause of size/shape segregation, namely mobility difference. As it does not consider actual particle interaction forces, it cannot be expected to match reality quantitatively in terms of real time or number of shakes. However, it is expected to predict the relative trend correctly, at least for free flowing mixtures.

When mobilities differ by a large amount due to a large size ratio, a situation previously identified as the percolation mechanism [14,27] occurs. Using arbitrary shapes, the pore spaces between particles can greatly increase. When combined with particles that have a much smaller diameter than the largest particles, as was the case for numerous mixtures investigated in this work, the chances that these particles are able to fill or pass through the voids with the aid of only small, externally applied taps greatly increases. For the experimental beds reported, therefore, the mechanism of percolation was observed to play a significant role in the early stages of segregation. When the fine particles were mixed throughout the bed, much of the segregation, which occurred initially, was caused by this effect, whereby the large particles acted as a screen as in sieving, through which finer particles could pass. In previous studies [14,27] this mechanism of segregation has been attributed to vibrations, where the bed of coarse particles is mainly static, with finer particles moving about a mean position. The few relative movements between particles can be attributed to the slow uplifting of the container. This was comparable to the conditions used in the simulations where there was no relative motion in the uplifting stage. The mechanics of percolation were clearer to see within some mixtures than for others in terms of the rate at which different mixtures segregated. As a whole, segregation required the fewest number of taps for the mixture consisting of CLG and FGS, two granular components, which in part thanks to the relatively large difference in size ratio and angular geometry provided the highest number of pathways for relative mobility. This mixture was closely followed by the pasta tubes and FGS in terms of ease of segregation, due to the fact that the elongated thin shapes allowed finer particles to pass, in addition to the smooth surface of the pasta tubes which provided minimum resistance. For mixtures with smaller size differences (i.e., pasta tubes and rice grains, pasta tubes/rice grains, and CLG), a greater number of taps were needed for segregation to occur, as the finer particles were unable to pass through the gaps created between particles within the respective beds without a degree of rearrangement occurring. For these mixtures, percolation was less obvious due to a combination of relative size and, especially in the case where both particles types

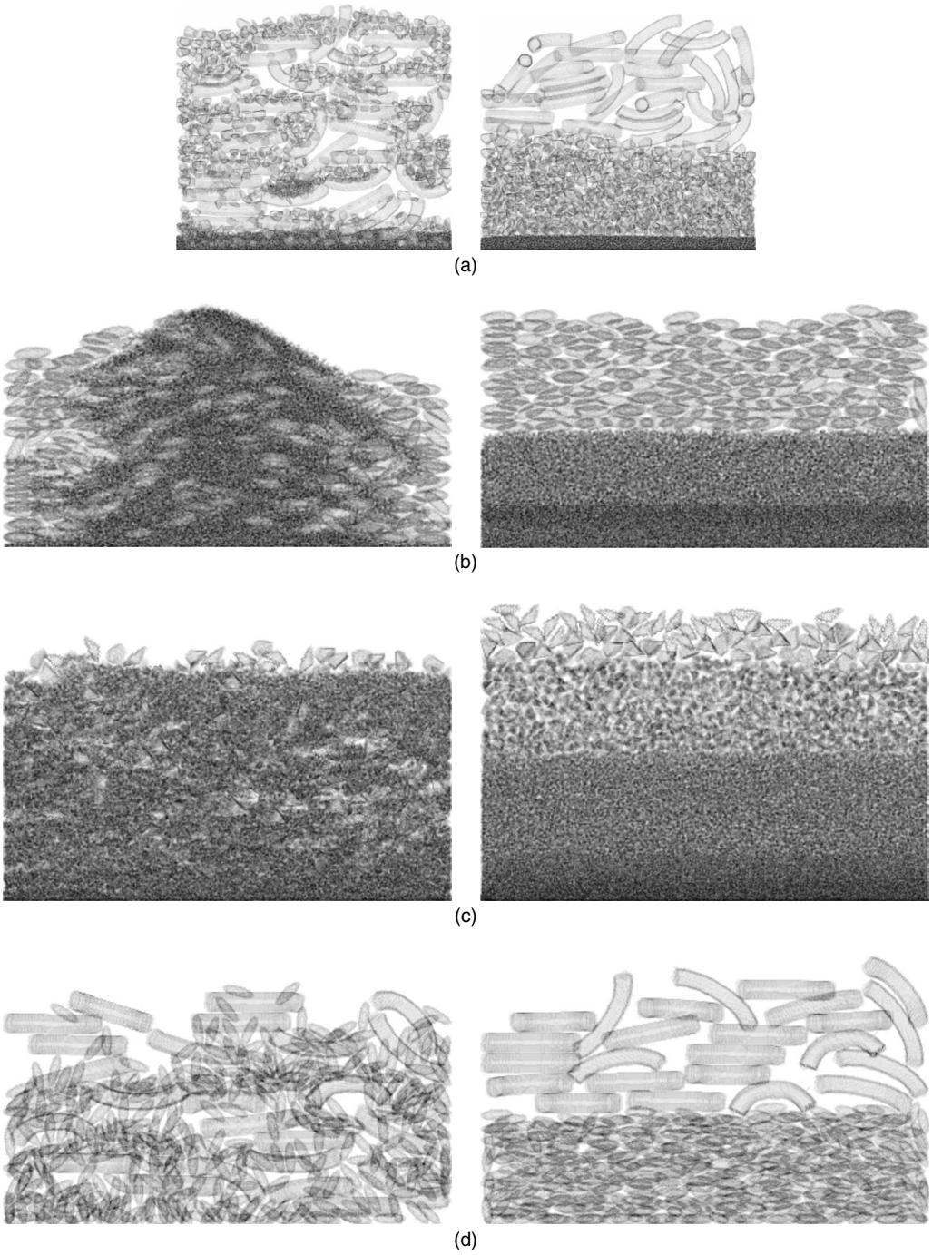

FIG. 6. Simulated beds of mixed (left-hand column) and segregated (right-hand column) beds corresponding to number of taps shown in Fig. 4. (a) Pasta/CLG, (b) Rice/FGS, (c) CLG/FGS, (d) Pasta/Rice.

display elongation, particle shape. Additionally, the ability of the pasta tubes to retain particles within their curved structure (Fig. 8), and for crushed limestone grit, which when mixed with components of similar size, the rough surface of individual grains, may also have contributed to the slower rate of segregation.

However, the mechanism of percolation, although observed in most of the mixtures, was the leading cause of segregation in only the initial stages of the tests. Once many of the fine particles had moved lower down the bed, other mechanisms then appeared to dominate in the segregation process. In the experiments, one type of segregation to occur that was not seen in the simulations was that of impact segregation. This is where two particles collide and the relative size of the particles defines how they react. For example, a large particle colliding with a much smaller one will not have much of an effect on the larger particle. The fine one, however, may be slowed down, brought to a standstill or receive a greater horizontal velocity in another direction. This is one of the causes of build up of fines at a container wall, as it causes fine particles to spread further. The fixed length random walks, which cause larger particles to move more

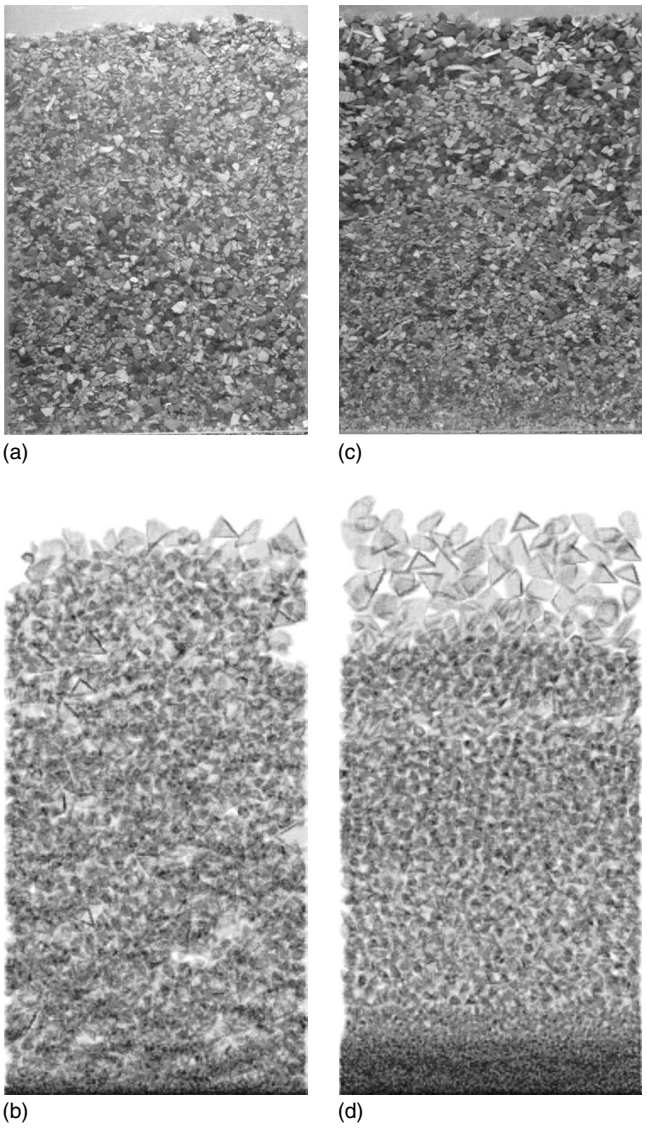

FIG. 7. Visual comparison of experimental and simulated beds of CLG corresponding to number of taps shown in Fig. 4.

slowly than smaller particles relative to their sizes, capture this mechanism in part; but miss the other part—friction. In DigiRWP simulated shaking, the bed is lifted *en mass*, and particle-wall friction is neglected. During resettling, particle-particle friction is accounted for only to the extent of surface roughness retained in the digitized particles, particle-wall friction remains neglected as in this case the container walls are flat and there are no protruded voxels to stop or hinder particle movements along the wall. The segregation mechanism that had the largest overall effect, seen in both the experiments and the simulations, was that of displacement segregation. Displacement segregation refers to the phenomenon where a large object initially buried at the bottom of a bed of small particles rises to the top as a result of vibration. Initially it was not very clear as the fine particles were distributed throughout the beds. As a greater proportion moved into the lower fraction of the bed due to percolation, however, displacement segregation gradually became more obvious. As the container was physically dragged down faster than the

FIG. 8. Entrainment of CLG particles within the packing matrix of the pasta tubes.

particles, it caused the particle assemblage in the container to separate from the base (approximately the height of the shaking amplitude) before falling back down. Any fine particles in this lower fraction then had the opportunity to move in below any coarse particles, preventing their fall before being subsequently "locked" into place. In other words, friction or particle-wall interaction has given rise to different mobility between particles near the wall and those in the bulk. It is also the cause of the convection mechanism for segregation, as has been described in [28].

The overall aim of running the simulations containing arbitrary particles was to investigate whether it was possible for the DigiRWP algorithm to mimic the experimental results in terms of the relative number of taps required to achieve segregation for various different mixture combinations. From Fig. 4, the number of taps required to achieve segregation (segregation index of 0.9) for all seven mixture types, in terms of measured and predicted results, are in qualitative agreement, with simulated beds requiring significantly fewer taps than those of the experiments. In addition, the predicted relationships between the relative mixtures (also in terms of segregation), are correlative in respect to the experimental results. As the simulation model used to obtain these results does not consider physical interactions, these results go some way to suggesting that segregation can be considered from a predominantly geometric point of view rather than the conventional mechanistic one.

Reasons for the large difference in the number of taps between measured and predicted results could be attributable to a number of conditions, either acting individually or in combination. The main reason is that DigiRWP is a fixed-length random walk based Monte Carlo method implemented in a relatively coarse lattice grid. Typically, digitized particles have dimensions (measured in pixels) ranging from tens up to a few hundreds. The fixed-length walks, which are one grid cell in length, are large compared with a dynamic model such as DEM where movement per time step would have been a tiny fraction of a pixel size. Thus, DigiRWP requires orders of magnitude fewer steps to simulate packing than a DEM model would. Another reason is the much smaller samples of mixtures used in the simulations than in

TABLE I. The combinations of the seven nonspherical mixtures investigated, and the total numbers of particles used in the DigiPac simulations. Simulation resolution was 0.25 mm/voxel.

Bed	Component 1 (coarse)	Component 2 (fine)	Total number of particles (simulation)
Mixture 1	Pasta tubes	Rice grains	421
Mixture 2	Rice grains	CLG	11868
Mixture 3	Pasta tubes	FGS	44025
Mixture 4	CLG		14440
Mixture 5	CLG	FGS	41593
Mixture 6	Rice grains	FGS	27120
Mixture 7	Pasta tubes	CLG	10531

the experiments. This is because to obtain the packing statistics for the respective beds, such as packing density, coordination number and orientation statistics, it is not necessary to perform a simulation that matches the real scale—several hundred to a few thousand particles are usually sufficient (Table I). Since the aim was to obtain a qualitative trend, this approach is therefore more cost effective and less restrictive than physical experiments, and much faster than dynamic simulations involving actual interparticle forces. Another possible contributory factor involves the simulation conditions. For example, one of the main difficulties in setting up the simulations was calibrating the shaking amplitudes and shaking intervals with those of the experiments, as the model has no direct link with real time. In the experiments it was observed that when the container was on a descending stroke, where it was dragged down faster that the bulk of the bed contained within, finer particles would move in beneath coarser ones before the base of the bed was compressed by the bulk above. The upper part of the bed, however, barely had time to settle before the following cycle of tapping occurred. Therefore, the upper few particles of the bed were never fully static. In the DigiRWP, conditions could be finely adjusted by means of the shaking interval and rebounding probability in an attempt to obtain a close visual match. However, one of the known problems with DigiRWP is that if the shaking is too frequent then some particles will remain suspended in the final configuration. Therefore, they do not have time to settle down before the next shake begins. Because of this, instead of moving downwards, these particles actually move up over time. The root cause is because DigiRWP does not consider real forces. For this reason, a longer tapping interval had to be used to ensure that all the particles moved downward in tandem, thus allowing the particles in the upper part of the bed time to settle, which may have had some influence on the number of taps required to achieve segregation. Additionally, other simulation conditions including the surface roughness of digitized particles, container shape and simulating wall effects, which are both interparticle and interwall related, could also potentially affect the simulation results in a way that is difficult to quantify. However, by keeping all variables constant from one run to another, apart from that of the different mixture components, it was possible to obtain results, which were qualitatively comparable with those of the experiments.

For a mixture of different sized/shaped particles, all that is needed for segregation is relative motion—it does not matter how that relative motion is achieved. Inter-particle and externally applied forces in the physical world, and rebounding probability constrained random walks in the simulated world, are merely means to generate relative motion. Fundamentally, from a geometrical perspective, mobility differences are the root cause of segregation. If this is true, then a geometrical packing model such as DigiRWP could prove useful for predicting if segregation is to happen and the relative rate at which mixtures of different compositions segregate under uniform conditions. 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. Thus, although the packing algorithm cannot be used to follow in detail the dynamic process of segregation, it provides a predictive means to help answer the fundamental questions of if and how likely segregation is to occur for any given mixture. A simple and fast procedure like this can therefore provide a versatile design tool of value to product formulators. However, although it is argued here that particle geometry, particularly of nonspherical media, is the determining factor in how different mixtures of particles behave when subjected to external forces, mechanical influences cannot be ignored completely, hence, only a qualitative analysis is undertaken.

V. CONCLUSIONS

From the description of the original DigiPac model (i.e., DigiRWP), it is clear that the geometrical packing algorithm was not designed specifically for the simulation of particle segregation. And yet, when used for multiple component mixtures of spherical and nonspherical particles alike, segregation is a natural outcome of using the packing algorithm.

More importantly, it is believed that the DigiRWP model captures the essential features of the segregation process, leading to interesting predictions that are found to be consistent when compared with physical experiments in both pseudo-2D and three dimensions. The most important advantage of the model is that it leads to a simple geometrical explanation of the rising mechanism, where it has been shown that DigiRWP is able to predict qualitatively the

correct trends for segregation in different types of mixtures. The number of cases in which this occurs precludes the possibility of a pure coincidence, and suggests that geometrical considerations alone may be used to explain and predict the tendency of segregation. The findings of this study demonstrate that, as dynamic particle interactions are not simulated, the resulting simulations where segregation is seen will be a consequence of the relative motion between particles of different shapes and sizes, regardless of the physical or mechanical causes of the relative motions.

It can be concluded that segregation is a phenomena, which is controlled to a great extend by the geometry of the objects. Different rules like particle L/d ratio, sphericity, and relative size ratio have a strong influence on the ease of segregation. The relative rates at which particles segregate depends on the efficiency by which smaller particles can occupy the voids created between larger particles. The easier it is for the particles to find and fill the void spaces, the faster the mixture will segregate. DigiRWP proves to be an effective tool for the study of segregation, and a simple and fast procedure such as this can be of practical use to product formulators in cases where it is desirable to know in advance the tendency for segregation among different formulation designs.

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