Comment on "Three-Dimensional Model for Particle Size Segregation by Shaking"

In a recent Letter [1] Jullien, Meakin, and Pavlovitch presented computer simulation results for particle size segregation by shaking. From their results they conclude that there is a minimum size ratio of about 2.8, below which segregation does not occur. However, *this result conflicts with well-established experimental facts [2]*, and is an artifact of using an ordered sequential algorithm to study granular motion. The shaking amplitude is commonly the control parameter in real segregation experiments [2], but the sequential simulations in [1] *cannot* include this dependence. We stress that collective effects, which have already been included in our simulations, are vital to describe many properties of vibrated powders [3], including segregation. The erroneous features in the results of [1] can be traced to (a) the sequential nature of their simulation method and (b) the lack of a stochastic element in their driving force (which models the effect of complex many-particle collisions).

(a) Cooperative motion is a *fundamental* property of the behavior of shaken powders including segregation phenomena. In other words, all the particles in a shaken powder are in motion simultaneously so that the nature and the duration of their relative motions *must* depend on the quality and amplitude of the driving force. These properties of the driving force must therefore be included in any realistic model of shaking. In the sequential process of [1] there is no real relative particle motion—any apparent cooperative behavior arises only from changing the order in which individual particles are moved. However, these changes in order can only be made *between* shake cycles and therefore they *cannot* be influenced by other elements of the vibration such as an amplitude. This is in conflict with experiments [2], which make it clear that amplitude dependence is an *essential* feature of size segregation by shaking.

For monosize spheres the ordered sequential algorithm used in [1] leads to steady-state structures which have volume fraction $\phi = 0.593$ and mean coordination number $z = 6.00$. By contrast our *nonsequential* algorithm leads to an explicit dependence of these quantities on amplitude with $0.55 < \phi < 0.64$ and $4.5 < z < 5.0$ [3]. As expected, this dependence then also appears in the transport properties of powders [4], in agreement with experiments [2]. *Nonsequential particle motion (which results in amplitude dependence) is an essential feature of the dynamical properties of powders, including size segregation phenomena, and this feature is precluded by the sequential algorithm of [1].*

(b) The minimum size ratio for segregation postulated in [1] results from the omission in [1] of a stochastic element from their shaking process. In reality the effect of shaking on granular materials is to change the configuration of the particles repeatedly [3]; *fluctuating* configurations are an essential feature of shaken powders and are not present in [1]. Using their algorithm a random close packed assembly of monosize spheres will relax into a configuration that is stationary with respect to further shakes, such as a roughly layered configuration. A large impurity sphere will only disturb this stationarity if its size is sufficient to cause a change in the deposition sequence at the next cycle—*the generation of unphysical, stationary configurations is thus the origin of the threshold for size segregation in [1].* For a roughly layered configuration the critical radius would be ≈ 1.5 times the layer spacing, or, roughly speaking, 3 times the small sphere radius (cf. the value 2.8 in [1]). This threshold does not exist in real segregation phenomena [2] and realistic simulations must preclude the stationary configurations which are its origin.

In our more sophisticated simulations [3–5], stationary configurations do not occur because of the incorporation of a stochastic element in the algorithm. *In accord with experiments [2] our results do not exhibit a size ratio threshold and they show a continuous variation of the single impurity sphere segregation rate for particle size ratios between 0.7 and 1.5.* To sum up, the results of our simulations [5], as well as those of experiments [2], do *not* support the existence of a size threshold for segregation phenomena.

The ordered sequential algorithm used in [1] is inadequate for describing the shaking of a powder and phenomena such as size segregation. This is because, without a stochastic element in their driving force, their ordering process leads to particle configurations which are stationary with respect to shaking *and hence to an unphysical size threshold for segregation.* In addition, because of the absence in [1] of nonsequential dynamics, the amplitude dependence of size segregation phenomena *cannot* be incorporated. This dependence is an essential feature of segregation experiments [2] and has already been incorporated in more sophisticated simulations [5].

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