Physica A 416 (2014) 279–289

Contents lists available at ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

Influence of particle shape and sample width on uniaxial compression of assembly of prolate spheroids examined by discrete element method

Piotr Parafiniuk *, Marek Molenda, Józef Horabik

Institute of Agrophysics PAS, ul. Doświadczalna 4, 20-290 Lublin 27, Poland

HIGHLIGHTS

- Uniaxial compression of assembly of spheroidal particles was examined.
- Influence of particles elongation and sample thickness was investigated.
- Volume fraction was found to change with thickness of the sample.
- Pressure ratio was found dependent on the aspect ratio of the particles.

ARTICLE INFO

Article history:
Received 16 December 2013
Received in revised form 6 August 2014
Available online 6 September 2014

Keywords:
Uniaxial compression
Discrete element method
Granular mechanics
Prolate spheroids
2D–3D transition

ABSTRACT

We use numerical simulations based on the discrete element method (DEM) to study the response of a cuboidal assembly of spherical (diameter d) or spheroidal particles to uniaxial compression. This study examines the influences of slight deviations from the spherical shape of particles or of the thickness of cuboidal samples on the packing and mechanical characteristics of the assembly. The spheroidal particles were fabricated by the multisphere method. Eight different particle shapes were considered, each with the same volume and with aspect ratios α from 1.0 to 2.5. The final vertical height and larger horizontal depth of the cuboidal deposit were $15d$, whereas the thickness ranged from $1.025d$ to $10d$. Upon increasing the assembly thickness or deviating from a spherical shape, numerical examinations by the DEM revealed clear differences in the packing structure and uniaxial compression of assemblies of spheroidal particles. The departure from a spherical shape results in intense changes in contact network, which is manifested as changes in the volume fraction, mean number of contacts per particle, and ordering of the deposits. For the more elongated particles, the pressure ratio as a function of spheroid aspect ratio reached nearly constant values regardless of the sample thickness.

1. Introduction

Numerous phenomena in nature and in industry involve particulate or granular materials. Since the early 20th century, this fact has driven research into these materials. In 1964, Bernal [1] published the results of an extensive and influential study of the structure of liquids that used physical models made of equal-sized ball bearings. In 1996, in a review of research developments, Jaeger pointed out that [2].

* Corresponding author. Tel.: +48 817445061x182.
E-mail addresses: pparafiniuk@ipan.lublin.pl, pparafiniuk@gmail.com (P. Parafiniuk).

http://dx.doi.org/10.1016/j.physa.2014.08.063
0378-4371/

> Over the last decade, there has been a resurgence in this field within physics. Sand piles have become a fruitful metaphor for describing many other, and often more microscopic, dissipative dynamical systems.

Investigations were conducted based on theoretical analyses, physical modeling, and following the increase in computing power, numerical modeling. Cundall and Strack [3] applied the discrete-element method (DEM) to numerically test 197 two-dimensional circular disks in an effort to reproduce the force network obtained in an earlier elastooptic experiment. Two-dimensional systems were further explored and compared with simulations based on disks or rods. Rothenburg and Bathurst [4] numerically simulated biaxial compression of assemblies of planar elliptical particles and concluded that their mechanical behavior did not significantly differ from that of assemblies of disks. The strength of assemblies of elliptical particles was comparable to those of real granular materials, whereas the strength of disk-shaped particulate assemblies was much smaller. Rothenburg and Bathurst claimed that most strength effects associated with assemblies of elliptical particles resulted from their higher density of contacts. A 5% increase in particle eccentricity typically added an extra contact per particle, and resulted in the peak friction angle increasing from 26° to 38°. Compared with particles of low eccentricity, particles of large eccentricity were observed to respond very differently to mechanical stimuli. Moreover, distinct differences were noted in the distributions of contact forces between circular and elliptical assemblies, with the latter exhibiting stronger contact anisotropy. O'Sullivan et al. [5] summarized earlier results, and by using a combination of discrete-element simulations and laboratory experiments, examined the changes in biaxial compression of rod assemblies in response to slight changes in the particle geometry and friction. A key finding was that the response of assemblies of hexagonally packed rods was very sensitive to minor changes in rod geometry. The peak friction angle decreased upon increasing the standard deviation in the distribution of particle–surface friction. The increase in computing power allowed systems of three-dimensional particles to be simulated: first monodispersed spherical particles and later polydispersed spherical particles or clusters of spherical particles (multisphere method). Some particulate materials encountered in practice are composed of cohesionless granules of relatively simple shape (e.g., agricultural seeds or plastic pellets) but, in general, particles may be of arbitrary shape and have a very wide distribution in size (e.g., granular fertilizers or instant soups). State-of-the-art numerical experiments have shown that some aspects of the mechanical behavior of particulate materials may be simulated by assemblies of spherical particles, while other phenomena or experimental conditions require a more accurate representation of the shape and surface properties of particles. On the basis of numerical simulations of a rotating horizontal drum, Walton [6] reported that at very low interparticle friction coefficient μ_{pp}, the angle of repose increased almost in proportion to the increase in friction coefficient. After exceeding 0.05, any further increase in friction coefficient produced only a very slight increase in the angle of repose. Walton also simulated nonspherical particles and concluded that no equivalent change in μ_{pp} existed that could make an assembly of spherical particles behave like an assembly of nonspherical particles. Moreover, Walton proposed that nonspherical shapes (or other effects not considered in previous work) were required to achieve angles of repose higher than approximately 31°.

To study the behavior of elongated particles, numerous experiments were done with ellipsoids or clusters of spheres [7]. Donev et al. [8] found that increasing the ellipsoid aspect ratio α (i.e., the ratio of the longer axis to the shorter axis) from 1.0 to 1.5 resulted in a sharp increase in relative density. They attributed this effect to an increase in the number of contact points that in turn were due to the additional rotational degrees of freedom of the ellipsoids. More contacts per particle were required for jamming, and forming more contacts required denser packing. Donev et al. [8] reported that the contact number appears singular for $\alpha = 1.0$ and rises sharply for small deviations from this value. Wiącek et al. [9] experimented with nearly spherical pea seeds and oblong beans and simulated the experiments by the DEM. They found that changing the particle shape from spherical to oblong (i.e., particle aspect ratio α increased from unity to 1.6) resulted in reduced porosity and an increase in specimen stiffness. Further increasing α to 2.8 resulted in reduced bulk density and a slight change in bulk stiffness. In addition, the particle aspect ratio was found to substantially influence the pressure ratio k. The change in particle shape from spherical to oblong resulted in significant decrease in lateral-to-vertical pressure ratio due to higher internal friction of oblong particles that resulted in lower k. Further increase in α beyond 1.6 produced only negligible changes in k. Apart from representing the shape of granules, the dimensions of simulated assemblies remains a question in itself. Assemblies should be as small as possible to reduce computation time or sometimes to enable efficient computation, but at the same time be large enough for the simulation to reproduce the behavior of real materials. The question is equally important for experiments where a representative elementary volume (REV) must be established. The REV is the smallest specimen whose measurement will yield a value representative of a large volume (deposit). Based on experience from numerous laboratories, the authors of Eurocode 1 [10] proposed that the diameter of a direct shear cell be 20 times that of the largest particle. Masson and Martinez [11] showed that a sample size seven to eight times the size of the largest particle was sufficient to obtain a macroscopically representative value for porosity and coordination number. To obtain a macroscopically representative value for the stress tensor, a sample size twelve times that of the largest particle was required. Wiącek et al. [9,12] used physical uniaxial compression tests and numerical simulations thereof to conclude that under the given conditions, a specimen of dimension greater than five times the particle size may be used as a REV. Börzsönyi and Stannarius prepared an extensive summary of recent progress in the understanding of packing, dynamics, and orientational ordering of granular materials composed of elongated particles [13]. They claim that "A quantitative understanding of the relationship between particle shapes and their behavior in macroscopic ensembles may thus have a substantial impact on technology and our control of natural processes". Another very significant factor in the laboratory or in nature is the confinement of granular assemblies in vessels made of smooth, rigid walls. This results in numerous effects that do not take place in the