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A study on the influence of particle shape and shape approximation on particle mechanics in a rotating drum using the discrete element method

D. Höhner *, S. Wirtz, V. Scherer

Department of Energy Plant Technology, Ruhr University Bochum, 44780 Bochum, Germany

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ABSTRACT

In this study experimental and numerical investigations with the discrete element method (DEM) on the mechanical interactions of spheres and polyhedral dices in a rotating drum are conducted. In DEM the dices are approximated by polyhedra and smoothed polyhedra respectively and hence allow examining the influence of sharply-edged and smooth particle geometries on the mechanical behavior. Simulation results are in good general agreement with the experiments and hence demonstrate the adequacy of DEM as well as polyhedral and smoothed polyhedral approximation schemes to simulate non-spherical particle geometries. It was observed that an increase of particle angularity leads to an increase of the dynamic angle of repose. On the other hand, while spheres mix faster than the polyhedral dices, no significant difference in the mixing behaviors of the dices can be observed.

1. Introduction

Granular materials can be found in various shapes and quantities in a wide variety of application areas such as the energy sector, the food and pharmaceutical industry as well as geophysics. Knowledge about the mechanical behavior of these materials is of major importance for a proper design of processing units such as silos, rotating drums and firing systems. Rotating drums in particular exhibit a wide range of phenomena such as avalanching, mixing and segregation that involve granular materials and are not fully understood yet.

The discrete element method (DEM), as introduced by Cundall and Strack in 1979 [1], has proven to be a capable tool for predicting the dynamics of large particle assemblies. A comprehensive overview about the major applications of the DEM in recent years is given in [2]. Several authors such as [3–6] identified particle shape approximation as one of the key challenges of DEM simulations, due to its significant influence on the mechanical behavior of granular materials. Nevertheless, most simulations conducted with the DEM involve spheres due to their simplicity in terms of contact detection, which results in lowest possible computing times. The major drawback of using spherical particle representation in the DEM is that most industrial granular materials exhibit a significantly different shape. As a result DEM predicts a deviating mechanical behavior on the single grain level as well as in larger particle assemblies, which renders the physical meaning of the obtained simulation results questionable [7].

For this reason several non-spherical particle shape approximation schemes have been proposed in literature. The most commonly used approaches include ellipsoids [5,8,9] and superquadrics [10–12], clustered-spheres approaches [13–15], polyhedra [16–19], sphero-cylinders [20] and discrete function representations [21,12]. Especially polyhedra pose an interesting option due to their flexibility to approximate arbitrarily shaped objects of both symmetrical and asymmetrical shape at various accuracy levels. Moreover it was shown by Höhner et al. [6] that polyhedra allow approximations of sharply-edged as well as smoothed particle shapes, further increasing its versatility.

In the following a brief overview over recent experimental and numerical studies on the influence of particle shape on the mechanical behavior of particle assemblies is given. Cleary and Sawley [13] investigated particle shape effects in 2D hopper flow using the discrete element method. In particular they studied the effect of both particle angularity and aspect ratio independently and together. It was shown that increasing angularity increases the flow resistance and reduces the flow rate of the hopper significantly while the flow behavior is only influenced moderately. On the other hand an increase of the particle aspect ratio not only reduces the flow rate in the hopper but also leads to substantial changes in the structure of the particle flow.

Cleary [22] conducted 2D DEM simulations of a Couette shear cell with elliptical particles of varying angularity and aspect ratio. Some of the major findings are that both angularity and aspect ratio lead to significant flow changes but a variation of the aspect ratio has the overall stronger effect. With an increase of the non-circularity the shear resistance of the granular material increases. Cleary attributes this to the ability of non-circular particles to interlock due to the presence of sharp corners, flat surfaces and higher numbers of contacts with surrounding particles. A similar effect on the particle–wall interaction could be observed, with non-spherical particles having an increasingly better grip on the walls resulting in a decline of the wall slip.

Markauskas et al. [5] investigated the piling of ellipsoidal particles and ellipsoids approximated with a multi-sphere approach in discrete

* Corresponding author. Tel.: +49 234 3223503; fax: +49 234 3214227.
E-mail address: hoehner@leat.rub.de (D. Höhner).

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element simulations. It was found that the piling behavior of the multi-sphere particles converges to the behavior exhibited by the ellipsoids with an increasing number of sub-spheres. They concluded that the multi-sphere approach is capable of approximating the mechanics of ellipsoidal particles with a reasonable number of sub-spheres.

Hilton et al. [23] carried out simulations on the pneumatic conveying of particles in a rectangular duct. The DEM simulations were coupled to the gas flow using a finite-difference code and showed that particle shape is critical to the transition between different flow modes. While particles with a high sphericity transition to slug flow at high gas flow rates, pronounced non-spherical particles transition to dilute flow. They explained this behavior with the smaller void fraction in the beds of non-spherical particles.

Mack et al. [24] conducted experiments and simulations with 322 spheres as well as a mixture of various polyhedral dices in hoppers of three different angles α. In 3D DEM simulations the dices were approximated as smoothed polyhedra, i.e. with rounded edges and vertices. The obtained experimental results showed that polyhedra flow is slightly faster than the flow of spheres and it was assumed that the flat surfaces enable them to slide past each other more easily. Moreover, for a hopper cone angle of $\alpha = 30°$, polyhedra showed a greater tendency for arching (based on two experiments performed per particle geometry and α). For a flat bottom hopper they additionally observed a higher tendency for polyhedral particles to pile up in the corner of the hopper. A reasonable agreement between experiments and simulations in terms of static packing, flow behavior and hopper discharge rates was accomplished.

Höhner et al. [6] also conducted experiments and simulations with spheres and polyhedral dices with varying sphericity in a hopper. In the DEM simulations the dices were represented as sharply-edged polyhedra and as smoothed polyhedra. With the exception of hexahedral particles they obtained a good general agreement between experiments and simulations with regards to discharge rate, flow profile and residual particle fraction in the hopper after discharge. In general they found that angular particles exhibit a lower discharge rate and a higher tendency to form pile-ups at the bottom walls of the hopper than spheres of similar volume and material. A comparison between both particle shape approximation schemes showed that sharply-edged particles lead to a higher increase of the microstructural strength of the particle assembly, which further enhances the effect of increasing particle angularity.

Although many studies on particle mechanics in rotating drums can be found in literature [25–29], the studies mentioned are mostly restricted to spherical particles. Kodam et al. [30] conducted experiments and DEM simulations of 250 acrylic glass cylinders in a rotating drum. They approximated the test particles as true cylinders in their DEM simulations and used a contact detection algorithm customized for cylindrical objects. A comparison of the mean dynamic angle of repose showed that DEM predictions lie within the uncertainty interval of the experimental results.

Wachs et al. [19] conducted DEM simulations of spheres and three different polyhedral particles in a rotating drum and examined the internal flow structure and the evolution of the dynamic angle of repose as a function of the rotation rate. They found that angular particles lead to an increase of the dynamic angle of repose as well as a loss of the flatness of the particle bed's free surface. In particular they found that the angle of repose increases with decreasing particle sphericity if the volumetric filling ratio of the rotating drum remains constant. Additionally they observed the occurrence of a slumping regime for non-spherical particles at low rotation rates where this could not be observed for spheres. The angular particle shape and the flat surfaces prevent particles from rolling down the free surface of the particle bed and promote avalanching, which results in an intermittent flow behavior.

In this study experiments and DEM simulations with non-spherical particles of varying sphericity in a rotating drum were conducted in order to evaluate the influence of particle shape and approximation accuracy on the mechanical behavior. For this purpose a laboratory scale rotating drum was constructed and differently shaped test particles were selected. The dynamic angle of repose and the mixing behavior were chosen as parameters characterizing the mechanical interaction within the rotating drum. Moreover the effect of shape approximation is analyzed by applying two different methods of approximating non-spherical particle shapes in the DEM.

2. Experiments

2.1. Test particles

For all experiments spheres as well as three different polyhedral dices were used (see Fig. 1). The polyhedral geometries are icosahedra, dodecahedra and hexahedra and exhibit a decreasing sphericity, i.e. increasing deviation from the spherical shape, in that order. For this reason they can be interpreted as sphere-approximations at different levels of accuracy.

The dices are made from acrylic glass (PMMA) and were dyed with car finish in two different colors (green, red) in order to allow studying the mixing behavior within the rotating drum. Note that the spheres consist of polyoxymethylene (POM), which has similar mechanical properties as PMMA, and were dyed in blue and red for reasons of availability.

Tables 1–3 summarize all relevant measurements, contact parameters and material properties of the test particles. A detailed description on how the particle properties were determined can be found in [6]. Note that we considered rolling friction in the DEM simulations only for spherical particles following Wang et al. [31] and Wachs et al. [19].

2.2. Test facility

For the experimental investigations a rotating drum as shown in Fig. 2 was constructed.

The rotating drum consists of acrylic glass (PMMA) and has an inner diameter of 290 mm (outer diameter: 300 mm) as well as a length of 500 mm. At the top a transparent PMMA cover plate was attached, allowing a view into the rotating drum during the test runs. Additionally, in the bottom wall a lockable opening was incorporated, which allowed filling particles into the rotating drum without previous dismantling. The drum is seated on 4 length-adjustable staffs, which are attached to a table plate at an angle of 45°. At the top of the staffs plastics rolls are fixated, thus allowing a rotational movement of the incumbent drum.

The rotating drum is driven by an electric motor, which is placed in a holding fixture underneath the table plate and can be vertically adjusted by a thread bar. A tooth belt is utilized to apply the torsional moment as well as rotational velocity from the rotating shaft onto the drum. A frequency converter regulates the driving speed of the motor and thus allows setting of the drum's rotational velocity. For additional inspection reflector stripes are fixed along the circumference of the drum, thus permitting to measure the rotational velocity of the drum with a laser control counter.

Table 4 summarizes the relevant boundary conditions for the conducted experimental and numerical investigations.

For investigating the mixing properties the particles were filled into the drum in two equally sized layers of red and green (blue) particles respectively as depicted in Fig. 3. Note that the number of particles differs between particle shapes as well as between experiments and DEM simulations (see Table 6).

Fig. 1. Test particles from left to right: sphere, icosahedron, dodecahedron, hexahedron.