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ORIGINAL PAPER

Simulation of the normal impact of randomly shaped quasi-spherical particles

Rimantas Kačianauskas · Liudas Tumonis · Algis Džiugys

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Abstract The paper reports the modelling of randomly shaped particles. An emphasis is placed on the illustration of random properties of particles, using simulations with a controlled probability distribution for the depth of the surface profile. The randomly-shaped quasi-spherical particles were described by applying a multi-sphere approximation and a statistical evaluation technique, and the surface of the particles was approximated using randomly located overlapping subspheres. The concept of statistically similar particles, i.e., particles characterised by having a similar probability distribution for the depth of the surface profile, was employed for these purposes, and an original method involving the application of a stochastic optimisation was developed. The optimization method was demonstrated by generating statistically similar particles. The contact behaviour was investigated by simulating a random particle impact against a wall, using the discrete element method. It was observed that statistically similar particles did not show statistically similar contact characteristics. The results of this study suggested that the refinement of the multi-sphere model (achieved by increasing the number of subspheres) was non-unique, not only in a deterministic context but also in statistical context, and that this subject requires further investigation.

R. Kačianauskas (✉)
Institute of Mechanics, Vilnius Gediminas Technical University, Basanavičiaus Str., 28, 03224 Vilnius, Lithuania
e-mail: rimantas.kacianauskas@vgtu.lt

L. Tumonis · A. Džiugys
Laboratory of Combustion Processes, Lithuanian Energy Institute, Breslaujos Str. 3, 44403 Kaunas, Lithuania
e-mail: liudas.tumonis@gmail.com

A. Džiugys
e-mail: dziugys@mail.lei.lt

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1 Introduction

The particle shape is an important property influencing the interaction of separate grains, and, in recent decades, many studies have been dedicated to improving the understanding of the role of the shape in the behaviour of granular materials.

Recently, the discrete element method (DEM), introduced by Cundal and Strack [1], has become the dominant computational tool for investigating the behaviour of granular matter. The DEM offers a direct way to numerically investigate the contribution of the shape, by computing the interactions between individual particles.

Because the solution of the contact problem for arbitrary shaped surfaces in three dimensions is complicated, a smooth sphere has become the most popular particle shape in DEM studies, and the explicitly defined Hertz solution for single sphere–sphere and sphere–plane contacts is extensively employed to simulate various particulate solids using the DEM.

In reality, the majority of granular particles are nonspherical, and may have irregular, randomly shaped geometries. Consequently, various models of varying complexity have been used to approximate such shapes. The existing DEM models for particles may be classified with respect to descriptors comprising the convexity and complexity of the shape (single or composite); the characterization of the global shape compared with a sphere, in terms of the sphericity, aspect ratio, or squareness; the sharpness of edges, in terms of angularity or roundness; and/or the smoothness (roughness) of the particle surface.

Earlier developments addressing the conceptual issues and the various computational aspects of the DEM relevant to the various possible shapes of particles are outlined in the review papers and references herein. We refer hereafter to reviews given by Herrmann and Luding [2], Džiugys and Peters [3], Latham and Munjiza [4], Cleary [5] and Wachs et al. [6], while relevant details will be mentioned below, where appropriate.

Considerable computational expenditure is required for the description of the contact geometry and the calculation of the contact points for arbitrarily shaped particles. Two basic approaches can be distinguished for the description of the particle surface for nonspherical particles. The first approach stems conceptually from monomer spherical models; the nonspherical particle shape is represented by a single smooth continuous scalar function. Ellipsoids, generalised super-ellipsoids [3], and super-quadrics [5,7] are smooth continuous shapes that have been explored in DEM simulations. This approach has the strong disadvantage that the detection of contact can generally only be achieved by iteratively solving sets of nonlinear equations. It is clear that shape models created using a single function are applicable for only a limited number of shapes, and are not suitable for irregularly shaped particles, especially those with sharp edges.

The second, composite approach approximates complicated real shapes by combining various regular shapes such as cutting planes, and cylindrical and/or spherical surfaces. This approach can be used to represent arbitrarily shaped, irregular, complex geometrical entities fairly well, but a different technique is required to describe the contact of particles.

A particular case of the composite approach was introduced by Cundall [8], and improved by Chen et al. [9], for polyhedral shapes, wherein convex particles were constructed using cutting planes. The advantage of using polyhedral shapes is that a wide variety of complex particle shapes can be simulated, meaning that more realistic results can be obtained from DEM simulations. However, the presence of sharp vertices complicates the treatment of particle contacts.

Another popular version of the composite approach is the multi-sphere (MS) method, in which the shape of nonspherical particles is constructed using rigidly connected, overlapping spheres. This method was introduced by Gallas and Sokolowski [10], and was developed in a systematic fashion by Favier et al. [11].

The most significant advantage of the MS approach is that it allows for an easy and efficient calculation of the contact between complex particles using only spherical contact models.

It was shown that, in contrast with models of perfect spheres, the MS method rendered a variety of particle shapes quite well, and allowed the essentially different behaviours of nonspherical particles to be distinguished [12–20]. The MS technique was successfully applied to deal with elongated particles, which were approximated by one-dimensional arrays of axi-symmetrically located spheres.

However, the axi-symmetric shapes were restricted to elongated spherocylindrical particles [14,17], and perfect ellipsoids [18]. Several studies aimed to model the irregular, complex shapes of geomaterials and other mineral particles using MS models, and illustrated the use of this concept with a modest number of subspheres [12,13].

A detailed comparison of both approaches, that is, the use of two-dimensional, regularly shaped polygons *vs* clumps of discs enveloped by identical circles, was given by Szarf et al. [21]. A comparison of polyhedral and MS models was presented by Höhner et al., wherein both models systematically converged on an enveloping sphere [22–24].

Recently, a hybrid spheropolyhedral approach was developed to accelerate the calculation of contacts between polyhedral particles. Here, a spheropolyhedron is considered as a polyhedron with rounded corners and edges. This approach was initially suggested by Pournin [25] for the simulation of complex-shape DEM particles. Discussions of later developments for convex spheropolyhedra were given by Wachs et al. [6] and Höhner et al. [24] (termed here as smoothed polyhedral), while the extension to the three-dimensional case for non-convex particles was described by Galindo-Torres et al. [26].

Several studies have attempted to apply the MS model to approximate regularly shaped smooth surfaces by further increasing the number of subspheres in a systematic fashion. Particular examples validating the use of the MS model to approximate elongated spherocylindrical particles were given by Abbaspour-Fard [17], and perfect ellipsoids were considered by Markauskas et al. [18]. A discussion of the approximation of non-smooth spherical particles using the MS model was given by Kruggel-Emden et al. [19]; it was shown that the application of the refined MS model could potentially change the macroscopic response. The authors assumed that the refinement of the particle model, which was achieved by increasing the number of subspheres, itself introduced additional errors.

The discussion of this issue was continued in later investigations [20–24], where the role of local non-convexity and multiple contacts, which lead to increased inter-particle friction and interlocking of particles, was emphasised. Höhner et al. [23] illustrated how the development of multiple contacts modifies the resulting force network. It is interesting to note that that refinement of the smooth ellipsoid shape via increasing the number of subspheres [18] yielded not a monotonic but a wavy variation in the contact number. The obtained results indirectly coincided with those obtained for agglomerates [27].

Omitting technical details, we focus here on the fundamental issues of the composite approach and the MS technique. Several tendencies can be identified, as detailed in this summary of our review:

1. Any modelled particle shape only represents an approximation of the real shape, independent of which numerical method is applied; therefore, the application of any method must be scrupulously justified.
2. The accuracy of the composite approximation of complex shapes can potentially be controlled and improved by increasing the number of discrete sub-elements, i.e. subspheres and/or planes, independent of which technique (MS, polyhedral or hybrid) is used to fit the shape of the particle as a whole.
3. The spherical approximation of the surface is preferable over a purely polyhedral approach with sharp edges, both from the computational point of view, and, in the majority of cases, for physical reality.
4. The above-mentioned studies have shown that the MS method is suitable for approximating the shape of particles on the scale of the particle size, and for improving the understanding of the features of non-spherical particles of granular materials, because it can link the macroscopic response with the micromechanical behaviours.
5. Paradoxically, an increasing number of subspheres in the MS model will not always lead to more accurate simulation results. Therefore, questions arise about the applicability and the limits of the MS model in the context of the smoothness (roughness) of the particle surface.
6. Because the shapes of real particles are characterised by high diversity and are of random character, a precise evaluation of the contribution of any individual particle shape is difficult to achieve; consequently, the deterministic approach contains random errors.

The literature shows how statistical methods can be used to describe granular behaviour based on the DEM simulations. The probability density functions of contact forces in a system of disks were considered by Kruyt and Rothenburg [28], while an investigation of the statistics and the correlations of forces acting on the walls under the pressure of poly-dispersed spherical particles was presented by Müller, Luding and Pöschel [29].

Among the various approaches to the simulation of non-spherical particles, the incorporation of the random factor and the available statistical data, in particular in combination with the advantages of spherical contact, offers an attractive alternative. This method has been explored by a number of researchers. A probability-based contact algorithm as an approximate method in statistics sense was presented by Jin et al. [30]. Here, contacts between nonspherical particles, were transferred into those between spherical particles with shape dependent contact probability. Random impact experiments were performed using a regular MS model [22], and the impacts of perfect spheres on a rough wall were described [31]. Generally, the non-smooth surface of a particle that is approximated by randomly located spheres may be treated using the contact mechanics for randomly rough surfaces [32,33]. However, the scale of the subspheres defining the non-smooth surface is different compared with that of the real asperities.

The problem of how to approximate real surfaces of particle has not yet been solved, and is still under discussion. Statistical data would therefore be useful in gaining knowledge of the random properties.

Our contribution addresses the micromechanical issue of approximating randomly shaped, non-smooth particle surfaces, and provides results obtained by combining the multi-sphere (MS) model and statistical indicators. The emphasis is placed on illustrating the contact behaviour of a randomly generated, multi-sphere particle with a controlled probability distribution for the depth of the surface profile. The geometry of the particle surface is considered in terms of a quasi-sphere composed of an arbitrary number of randomly located, rigidly connected, overlapping subspheres. The randomly-shaped particle was therefore considered as a quasi-sphere, while the particle-wall contact was investigated via DEM simulations of random impact experiments.

The paper is organised as follows: The concept of the model for the randomly shaped surface of a particle, and its statistical characterization, is given in Sect. 2. The method used to generate statistically similar particles is presented in Sect. 3. The DEM approach used for simulating the impact of randomly shaped particles on the wall is briefly described in Sect. 4. The statistics for contact variables obtained from the discrete element simulations are described and discussed in Sect. 5. Finally, concluding remarks are given in Sect. 6.

2 Concept and characterization of the particle

The simulation of particles requires knowledge of their geometry. In this section, a concept for a randomly shaped particle is described. It was assumed that the particle under consideration was of a quasi-spherical shape (Fig. 1). The geometry of a particular particle was related to an enveloping sphere with radius R. Consequently, it was assumed that the particle surface area A and volume V, as well as the mass and inertial moment, were equal to those of the enveloping sphere.

An approximation of the surface of the quasi-spherical particle was applied using an MS method, as follows. The MS approach implies that a quasi-spherical particle is composed of an arbitrary number N of rigidly connected overlapping

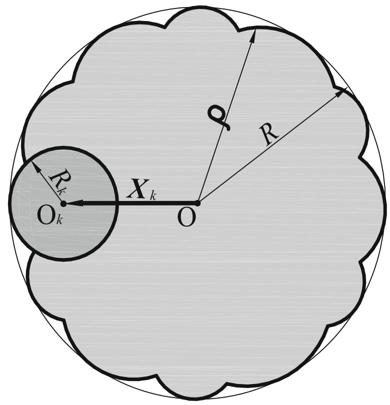

Fig. 1 Schematic view of a randomly shaped quasi-spherical particle

spheres, typically termed as subspheres, each of which is denoted by a subscript $k(k = 1, \ldots, N)$.

To formalise the arrangement of subspheres in a systematic fashion, the surface of the enveloping sphere was covered by a triangular grid containing N nodes. The centre O_k of subsphere k was located on the line connecting the enveloping sphere centre O with node k of the grid.

In the framework of this approach, the geometry of a quasi-spherical particle was controlled by the number of subspheres N, and the geometric parameters of the subspheres; namely, the radius of a subsphere R_k, and the position of a subsphere, as defined by a vector $\boldsymbol{X}_k$ pointing from the particle centre. Details of the particle geometry are presented in Fig. 1, where the quasi-spherical particle is represented by the shaded solid area. To characterise the resulting constructed surface of the particle, the surface was described in spherical coordinates; i.e. each arbitrary point on the surface was defined by the variable radius $\rho(0 \leq \rho \leq R)$ and the two spherical angles φ and ψ, varying within the limits $(0 \leq \varphi \leq \pi)$ and $(0 \leq \psi \leq 2\pi)$.

The non-smooth surface of the particle presented in a polar form was convex; i.e. each ρ was uniquely related to a single point on the continuous surface.

The surface profile of a quasi-spherical particle was characterized by the surface depth, which represented the radial difference between the enveloping sphere and the actual profile:

$$z(\varphi, \psi) = R - \rho(\varphi, \psi) \quad (1)$$

The surface depth was considerably smaller than the sphere radius; $z(\varphi, \psi) \ll R$. The mean value of z, obtained by numeric integration over the surface of the particle, was

$$z_{mean} = \frac{1}{A} \int_A z(\varphi, \psi)\, dA. \quad (2)$$

Various measures may be employed for the characterization of a non-smooth (rough) surface. We assumed that the surface of the quasi-spherical particle approximated by the MS model could be considered as rough [32]. There were no protrusions or dents deeper than the radius of the sub-spheres. Therefore, the mean surface depth z_{mean} defined by Eq. (2) was used as a main roughness parameter.

3 Multi-sphere model of the quasi-spherical particles

Our task was to investigate the contact behaviour of the statistically similar particles. Statistically similar quasi-spherical particles of radius R approximated by the MS model had a randomly shaped surface, whose profile was characterised using similar probability distribution depths. The surface depth was characterised in a discrete manner using a set of $z_j(j = 1, \ldots, N_{bins})$ values, where N_{bins} stands for the number of discrete intervals (bins). The probability distribution was represented as a histogram of the tabulated frequencies $p_j(z_j)$ of the observations.

Two types of particles, termed hereafter as regular and irregular particles, were used in our numerical experiments. The regular particle was generated using equal subspheres having the specified radius R_k for each node k of the grid, while random properties were imposed by the randomly specified distance $|\boldsymbol{X}_k|$.

A regular, relatively fine reference particle composed of $N = 300$ subspheres having a radius $R_k = 0.2R$ was used as the reference particle (Fig. 2a). The distance $|\boldsymbol{X}_k|$ was defined randomly within the limits of $R - 0.05R \leq |\boldsymbol{X}_k| + R_k \leq R$.

The probability distribution of the surface profile depth, as defined by Eq. (1) and scaled by the radius R, is shown Fig. 2b; it was characterised by the mean value $z_{mean} = 0.027R$.

The irregular particles had a much higher degree of randomness, and were generated using a random subsphere radius, R_k, as well as a randomly defined location for the subsphere centre point, $\boldsymbol{X}_k$.

For the numerical experiments, four sample sets of irregular quasi-spherical particles consisting of $N = 160$, 100, 80, and 40 subspheres (Fig. 3) were generated in such a way that the probability distributions for the surface profile depth of the reference particle and the sample particles were as close as possible. To achieve this similarity, the stochastic optimization problem was formulated, and a heuristic random optimization procedure [34] was used to generate the irregular particles.

The optimisation problem was formulated to find a set of discrete values z_j of the profile depth of the particle that minimised the goal function

$$g(z) = \sum_{j=1,N_{bins}} \left| p_{j,ref}(z_j) - p_j(z_j) \right| \rightarrow \min, \quad (3)$$

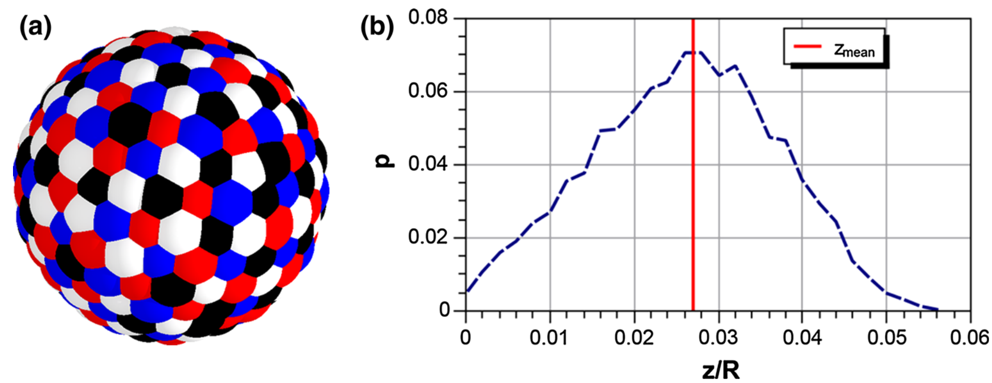

Fig. 2 Reference particle consisting of 300 subspheres: **a** geometry, and **b** distribution of probability of the profile depths, where $z_{mean} = 0.027R$

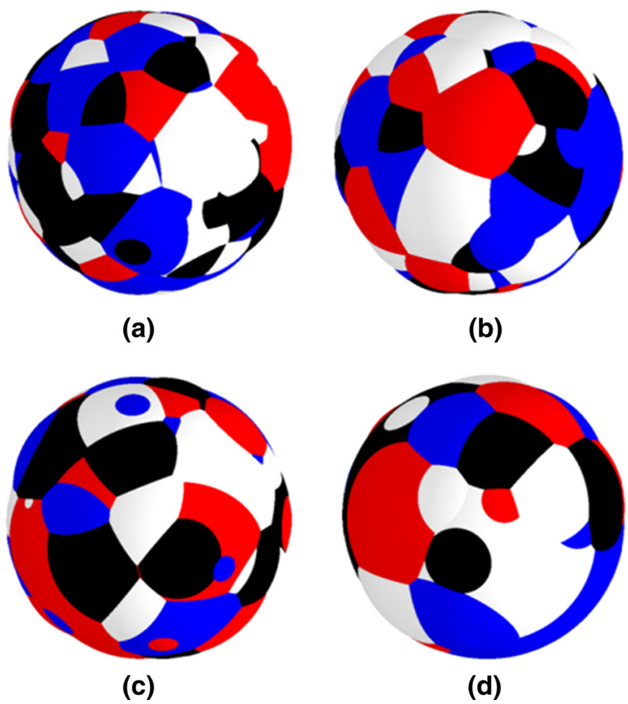

Fig. 3 Geometry of randomly shaped particles with $N = 160$ (**a**), $N = 100$ (**b**), $N = 80$ (**c**) and $N = 40$ (**d**) subspheres, respectively

giving the differences between the histograms for the designed sample particles and the reference particle. The goal function (3) is expressed in terms of the difference of probabilities between the reference and generated particles profiles, $p_{j,ref}$ and p_j, respectively. The quality variables $z_j(R_{jk,}, \boldsymbol{X}_{jk})$ were subjected to inequality constraints to provide reasonable limits for the set of primary variables R_{jk} and $\boldsymbol{X}_{jk}$, to maintain the integrity of the quasi-spherical particles.

Compared with classical deterministic optimisation methods, the most distinguishing feature of random optimisation is that a random effect is introduced during the search procedure. Thus, the search sequence for z_j was not determined only by specifying the z_j values, but also by the random factor that was introduced. The random optimization comprised

Table 1 Basic data of the generated particles

Sample	Reference	a	b	c	d
Number of spheres (N)	300	160	100	80	40
Normalized $z_{max} \times 10^{-2}$	5.80	5.73	6.33	5.79	6.18
Normalized $z_{med} \times 10^{-2}$	2.69	2.68	2.69	2.70	2.68
Histogram error (%)	–	1.21	1.17	0.51	1.68

the initial generation of a Gaussian random number vector of variables, and the step-by-step modification of function (3) using a random-trial check procedure, which involved a comparison of the objective function value for the previous point and a new trial value; the new trial value could either be accepted as a new point, or simply rejected. The final geometry was selected using the values of quality variables that yielded the best fit to the optimality criterion.

The simulation results for each particle comprised the normalized surface depth parameters, and histogram errors defined by the values of the goal functions $g(z)$; these values are given in Table 1.

The graphs in Fig. 4 show the probability distributions of profile depths for the sample particles; the vertical line shows the mean value of z. It is clear that the perfect statistical similarity, i.e., identity of the curves, was not achieved for the $p(z)$ distributions. However, the difference between the curves was insignificant; the maximum histogram error was only 1.68 % (Table 1). The generated reference and sample particles were used in further numerical experiments, as described below.

4 Impact simulations

The contact behaviours of the generated reference particle and four sample quasi-spherical particles (Figs. 2a, 3) were studied numerically by conducting normal particle-wall impact tests in the absence of gravity. Ten thousand random impact experiments were simulated for each particle using

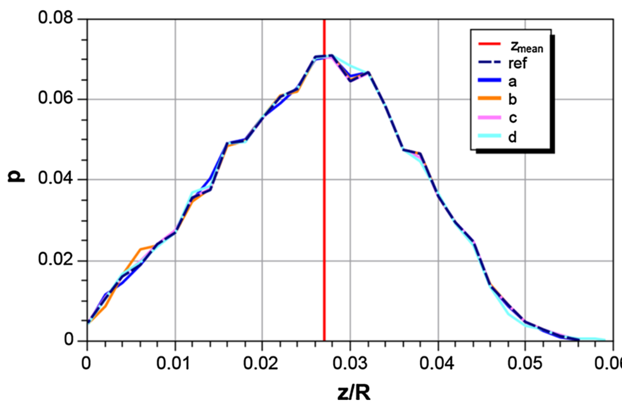

Fig. 4 Probability distributions of profile depths for the sample particles

DEM. Because gravity was excluded, only one particle-wall impact was simulated during each experiment. In each experiment, the initial impact velocity $v_0 = 1$ m/s was kept constant, and the initial rotation velocity was zero, while the initial orientation of the particle was set randomly using a white noise distribution of φ and ψ in the limits $(0 \le \varphi \le \pi)$ and $(0 \le \psi \le 2\pi)$.

The DEM methodology was used previously to simulate the dynamic behaviour of non-cohesive frictional visco-elastic three-dimensional multi-spherical particles [18], and this approach was applied in this study.

The motion of the particle as a rigid body in a time t was described in the framework of classical mechanics, and obeyed Newton's second law. The rotation of the sample particles and the reference particle was calculated in the same way as for a spherical body. All loads and torques acting on the particle during contact were transferred to the particle's centre via individual subspheres.

For a subsphere k belonging to the particle and contacting with the wall, the forces and torques were denoted by the vectors $\boldsymbol{F}_k$ and $\boldsymbol{T}_k$. Consequently, the resulting particle force and torque vectors $\boldsymbol{F}$ and $\boldsymbol{T}$ were the sum of all forces and torques $\boldsymbol{F}_k$ and $\boldsymbol{T}_k$ transferred to the centre of the particle:

$$\boldsymbol{F} = \sum_k \boldsymbol{F}_k; \ \ \boldsymbol{T} = \sum_k \boldsymbol{T}_k. \tag{4}$$

Here, the summation of torques in the above expression was performed for the torques with respect to the centre of mass of the whole particle. The above expression also includes torques that arose from the forces $\boldsymbol{F}_k$ acting on the subspheres. The vectors $\boldsymbol{F}_k$ were decomposed into normal and tangential components. The normal component $\boldsymbol{F}_{n,k}$ of the force vector $\boldsymbol{F}_k$ comprised a nonlinear elastic force following the Hertz model, and the damping force. The tangential force $\boldsymbol{F}_{t,k}$ was defined by elastic and damping components; it followed Coulomb's friction law during sliding. The elastic force was the Hertz force $\boldsymbol{F}_{n,el} = \left|\boldsymbol{F}_{n,el,k}\right|$ which was nonlinearly related to the particle–plane overlap depth, δ, as follows:

$$F_{n,el} = K\delta^{3/2} \tag{5}$$

Here, $K \equiv K_{n,k}$ represents the contact stiffness expressed in terms of the effective contact elasticity modulus E_{eff} and the effective radius of curvature R_{eff}.

$$K = \frac{4}{3} E_{eff} \sqrt{R_{eff}} \tag{6}$$

Thus, the effective elasticity modulus of the particle-to-plane contact in the case of the elastic plane substrate was $E_{eff} = E/2(1-\nu^2)$, where R_{eff} is the effective radius of curvature of surface of particle at the contact point, ν is Poisson's ratio, and E is the elasticity modulus. Rolling effects were neglected.

During contact, the equations of motion were integrated by applying a Verlet numerical integration scheme. The time step used for the integration was chosen as a constant $\Delta t = 10^{-7}$ s, so that the contact between the particle and the wall was resolved within 100 time steps. The developed method was implemented in the DEM code PARTCONTSTAT.

Each particle considered here had identical material properties. A particle was considered to be a homogeneous isotropic elastic body with the prescribed deterministic elasticity constants. The properties of fused silica—characterised by an elasticity modulus of $E = 71$ GPa, a Poisson's ratio of $\nu = 0.17$, and a mass density of $\gamma = 2200$ kg/m^3—were imposed to characterise the material properties of the sample particles used in our investigation.

Damping effects and friction were neglected. The normal impact of a particle with an elastic wall having properties identical to those of the particle was considered; the effective elasticity modulus was therefore $E_{eff} = 36.55$ GPa.

The particle radius R was 2.5 mm. For all of the sample particles, the mean surface depth was approximately $z_{mean} = 67.5$ µm, i.e. $0.027R$. The particle mass m and the moment of inertia I were calculated as the values for a perfect sphere with radius R, and values of $m = 1.44 \cdot 10^{-4}$ kg and $I = 3.6 \cdot 10^{-10}$ kg $\cdot$ m^2 were obtained.

5 Numerical results and discussion

Selected results from the numeric simulations characterizing the normal contact behaviour are presented below. Our discussion focuses on the performance of the MS approach, and its suitability for describing a non-smooth surface by applying the simplest statistical measures. It is clear that the contact between particles having smooth analytical shapes was uniquely defined by the deterministic relationships. Because the shape in the vicinity of the contact zone was of a random character, we also expected that the contact behaviour would be of a random character, and would reflect the properties of the data. The primary idea was to study the quality of our approach; i.e. to demonstrate quantitatively statistical relationships, if they existed. The statistical similarity between the properties meant that different particles with similar, i.e. almost equal, statistical characteristics exposed similarities between the statistical characteristics of the contact variables. It should be noted we restricted ourselves with respect to the data by controlling only the statistics for the depths of the surface profile.

The numerical study of the normal contact behaviour focused on the statistics for the multiple contacts, the contact force, and the contact duration, which were obtained by simulating the impacts in a normal elastic particle-wall experiment, where contact was initiated by the random orientation of the particle.

Because of the deviations of the surface away from that of a perfect sphere, considerable differences were observed in the contact behaviour, compared with perfect normal contact. First, we discuss the behaviour of the particle in the case of a single contact. In the case of a smooth sphere impacting a plane, contact started and continued at the single point; the contact was central, and was characterised by a probability $p = 1$. The contact force was defined by Eq. (5), while the stiffness in Eq. (6) was defined by the effective radius $R_{eff} = R$, which was equal to the radius of a perfect sphere.

For a given impact velocity v_0, the maximum displacement δ_{max} for Hertz's contact law is estimated as [3]

$$\delta_{max} = \left(\frac{25m^2}{2K^2}\right)^{\frac{1}{5}} v_0^{\frac{4}{5}} \tag{7}$$

while the contact duration is estimated as

$$T_c = 188\left(\frac{25m^2}{2K^2}\right)^{\frac{1}{5}} v_0^{-\frac{1}{5}} \tag{8}$$

However, the contact behaviours of the MS particles were different. Even in the case of a single contact they initially touched the plane through a subsphere k, which had a smaller radius $R_k < R$. The effective radius R_{eff} in Eq. (6) was then replaced with the radius of a subsphere R_k. Denoting variables relevant to the full particle contact using the subscript p, and variables relevant to particle contact via a subsphere using the subscript s, we could write explicit evaluations for both cases. It is easy to discern from Eq. (7) and Eq. (8) that a reduction in the contact radius increased the maximal displacement $\delta_{s,max} > \delta_{p,max}$ and the contact duration $T_{c,s} > T_{c,p}$. In contrast, it follows from Eq. (5) that a reduction in the contact radius reduced the contact force, and so $F_s > F_p$.

The second feature of the MS contact behaviour might have been related to the contact mode, because during collisions the particles with a non-smooth surface came into contact with the wall in a different manner; the impact was not necessarily central, and rotational motion might have occurred. We found that in our samples the contribution of the rotational energy was insignificant, and was therefore not analysed here.

The most significant feature observed in the behaviour of the MS particles was the presence of multiple contacts. Contact might have occurred at several contact points at the arbitrary instant of the particle collision. The number of multiple contacts might even have increased during the contact because of the deformation of the particle surface.

During normal impact, the motion of the particle over a time t was driven by the displacement $\delta(t)$, while the evolution of the force was obtained by tracing the displacement history. The occurrence of new contacts was taken into account automatically; however, the validity of energy and momentum conservation had to be properly controlled. In the case of multiple contacts, the characterisation of the particle behaviour was complicated, and could not be estimated in advance. Details on the multiple contacts occurring during a collision are discussed by Kruggel-Emden et al. [19], Kodam et al. [20] and Höhner et al. [21]. Selected results from the numerical simulation characterizing the normal contact behaviour are shown in Figs. 5, 6 and 7, which give histograms of the probabilities.

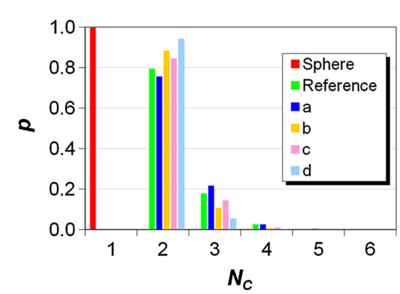

Fig. 5 Probability distributions of number of contacts N_c for different particles

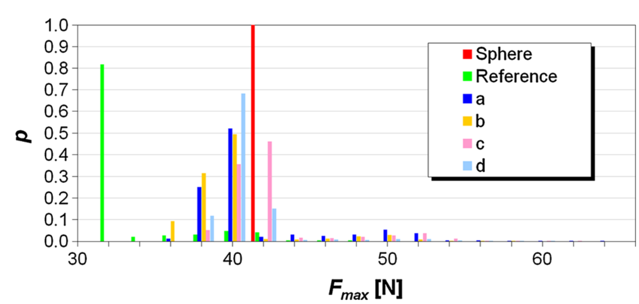

Fig. 6 Probability distributions of the maximum contact force F_{max} for different particles

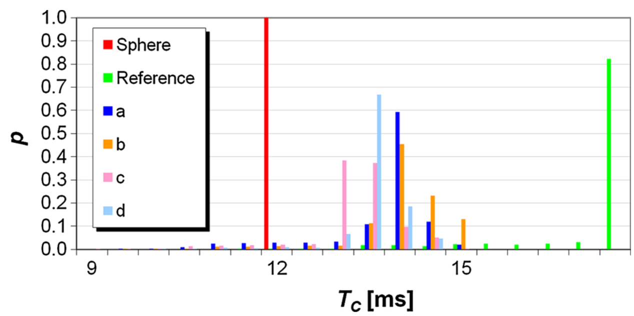

Fig. 7 Probability distributions of the contact duration T_c for different particles

Table 2 Summary of simulation results for different particles: average values of the maximum contact forces and the contact durations

Variable	Samples				
	Reference	a	b	c	d
$F_{\max}$ (N)	32.17	41.24	39.76	42.08	40.49
T_c (ms)	16.70	13.70	14.05	13.23	13.55

Here, the columns denoted by a, b, c and d indicate randomly generated particles having $N = 160$, 100, 80 and 40 subspheres, respectively. The column denoted as "Reference" indicates the reference particle. The column denoted as "Sphere" indicates the perfect sphere characterised by a probability $p = 1$; this column is shown in the histograms for the sake of comparison.

The probability distributions of the number of contacts N_c for different randomly shaped particles are shown in Fig. 5. They illustrate the occurrence of the multiple contacts. For our relatively stiff material, the maximum number of contacts was 5.

Probability distributions of the maximal contact force F_{max} and the contact duration T_c are shown in Figs. 6 and 7, respectively. A remarkable deviation was observed for larger forces (and for reduced contact durations).

Qualitatively, the histograms reflected the differences between the deterministic single contact approach and the distributed (i.e. multiple-contact) approach, in terms of the probability distributions. The simulation results are summarised quantitatively in Table 2, where the average values of the maximum contact forces and the contact durations extracted from numerical experiments are presented.

The numerically obtained results for the four generated irregular shaped sample particles showed scattering in the average values (see Table 2, columns a–d). The largest difference between the average values for the maximal contact force F_{max} was 5.83 %, while the largest difference between the contact durations T_c was 6.20 %.

The probability distributions of the contact variables for each sample were clearly quite different, and they were characterised by relatively large scattering in the values for the contact variables. Moreover, the sequential increase in the number of subspheres was only partially reflected by the statistics for the contact variables. Based on the results of the numerical simulation, it could be stated that the expected statistical similarity between the particles governed by the sequential increase of the number of subspheres was not retained for the contact variables.

6 Concluding remarks

The problem of approximating the randomly shaped surface of a quasi-spherical particle was considered by applying the multi-sphere model, and a statistical evaluation technique. Four quasi-spherical particles having probability distributions for the surface profile depth similar to a specified reference particle were generated using a stochastic optimisation procedure. The contact behaviour of particles was considered by conducting random impact experiments using DEM. It was observed that particles with statistically similar surface profiles did not show statistical similarity in their contact characteristics. The results of this study suggested that the dependency of the contact properties on the refinement of the multi-sphere model (achieved by increasing the number of subspheres) was non-unique, not only in a deterministic context, but also in statistical context, and that this subject requires further investigation.

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