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Investigation of rice grain flow by multi-sphere particle model with rolling resistance

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Abstract A multi-sphere (MS) model combined with rolling friction was considered for modelling elongated particles of irregular shape. The performance of the model was investigated by numerical simulations of the rice grain flow. A set of 5000 poly-dispersed milled rice grains were selected for the investigation purposes. They were characterised by a constant aspect ratio 3.5, while their maximum size was ranging from 6.4 to 7.3 mm. Filling and discharge flow as well as piling were simulated numerically with and without rolling resistance of particles. Simulation results were validated on the basis of experimental results. Good agreement of numerical and experimental results in terms of the discharge time and repose angle of the pile was reached simultaneously, when rolling resistance was introduced.

Keywords Discrete element method · Multi-sphere model · Rolling resistance · Experimental validation · Piling

1 Introduction

Granular materials containing nonspherical particles play an important role in various industrial applications. Flow behaviour of such materials is determined by the interaction of individual grains whose the experimental investigation at grain level is extremely difficult. However, the application of numerical simulations provides a feasible alternative to physical experiments. The Discrete Element Method (DEM) was recognized to be a numerical tool for simulating granular material after the publication of the Cundall and Strack [1]. In recent years, numerous authors have used the DEM to simulate the motion of grains and powders.

It is commonly agreed that the shape of the grains strongly contributes to the global response of granular solid. The shapes of non-spherical particles used in DEM simulations may be roughly classified into two categories: single-particle models and multi-particle models. The single particle approach considers a particle as a single body of complicated geometry. Smooth convex surfaces, such as ellipsoids [2] or superellipsoids [3], described by a scalar function as well as convex polyhedral [4], are the most thoroughly explored particle shapes. Recently, special attention has been given to more complex geometries, and various particle shapes have been developed by combining intersecting regular models. Generalised spheropolyhedra, resulting from smoothing sharp edges with spherical cylinder [5], present the convex shapes of this category.

In the second approach, a single non-spherical particle is represented by a composition of bodies. A multi-sphere (MS) approach presents the case of composite particle, therewith, a single non-spherical particle is represented by a composition of the bonded spheres or clumps. Representation and description of axi-symmetrical non-spherical particles by the MS model is presented by Favier et al. [6]. Several reported applications of multi-sphere models are agricultural axi-symmetric particles with high aspect ratio [7]. Two overlapping spheres were used by Zhou and Ooi [8] in simulating granular piling. Differently shaped clumps of spheres presenting primary non-spherical agglomerates were elaborated by Khanal et al. [9] and applied for simulation of fragmentation of composite discs.

One of the most serious problems, associated with the MS approach is, however, the lack of knowledge about the number of subspheres needed for the approximation of a real particle. Krugel-Emden et al. [10] studied spherical

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particles, approximated with a varying number of sub-spheres. A comprehensive study of adequacy of multi-sphere approximation for elliptical particles is presented by Markauskas et al. [11].

Generally, the particle properties required for DEM simulations may be obtained by the grain level experiments. However, for technical reasons, only macroscopic parameters of granular samples are measured in the majority of experiments. Even indirect extraction of the particle elasticity or friction parameters is not straightforward.

To approximate the reality with reasonable computational expenses, various simplifications are employed. They include the change of the material properties to increase the time step length [12], the reduction of the number of particles by scaling the size of the irregular particles, the simplification of the particle shapes etc. Consequently, the validation and/or calibration of the grain level parameters and contact models by conducting an experiment or parametric simulation is required to reflect the reality, see [12,13].

The paper addresses the capability of the MS particle model to be applied to DEM simulation of irregular particles. Thereby, the rotational symmetry is combined with rolling friction. The rice grain flow was simulated numerically and observed experimentally during the processes of hopper discharge and pile forming.

It should be noted that DEM simulation of the real agricultural particulate materials and rice grains, in particular, is not new. The most popular spherical particles are considered in [14,15], while spheropolygons are used in [16].

Accurate implementation and maximum adequacy of 3D DEM modelling to the experiment is manifested. The validation of the tangential and rolling friction coefficients by simultaneous matching of numerical and experimental results in terms of the two parameters, discharge time and repose angle of the pile, is considered.

2 Simulation methodology

The DEM methodology considered in this paper aims to simulate the dynamic behaviour of the rice grains represented by the non-cohesive frictional visco-elastic dry 3D elongated axis-symmetric particles. It is based on the conventional approach originally proposed to spheres by Cundall and Strack [1] and on the multi-sphere approach presented by Favier et al. [6].

The rice grain is presented by axi-symmetric MS model [11]. This model approximates an elongated axi-symmetric particle, such as ellipsoid or superellipsoid, by an arbitrary number of inscribed spheres. To control the size of the particle and minimize shape distortions, the model contains a central sphere. The spheres bonded with each other are located on the axis of symmetry.

The motion of an arbitrary particle i in time t as a rigid body is described in the framework of classical mechanics and obeys Newton's second law of motion.

The contact of multi-sphere particles is described via the contacts between separate spheres. Contact loads $\mathbf{F}_{ik}$ and torques $\mathbf{T}_{ik}$ acting on the particular sphere k are defined with respect to their center. Consequently, the resulting force and torque vectors $\mathbf{F}_i$ and $\mathbf{T}_i$ of the particle i (Favier et al. [6]) are the result of transferring $\mathbf{F}_{ik}$ and $\mathbf{T}_{ik}$ to the centre of the particle. Additionally, the gravity force is added to the centre of the particle.

Each component of the sphere force $\mathbf{F}_{ik}$ presents the resultant of contact forces with all colliding neighbour spheres. Each contact force acting between two spheres k and l, belonging to different particles, is decomposed into the normal and tangential components $\mathbf{F}^n_{kl}$ and $\mathbf{F}^t_{kl}$, respectively. A normal force is computed as the sum of the elastic force, following the Hertz model, and the damping force, defined by the Tsuji model [17]. Below Coulomb limit, which is characterized by static tangential friction coefficient μ, the tangential force is obtained similar to the way of obtaining the normal force, see [18,19]. During a gross sliding, the tangential force follows the Coloumbs friction law, retaining the fixed value of μ. More extensive reviews of contact models are given by Luding [20] and Zhu et al. [21].

The torque $\mathbf{T}_{ik}$, acting on the sphere k, comprises the contributions of all contacts. A particular torque component $\mathbf{T}_{kl}$ generated from two spheres depends on the constitutive model. In a conventional model proposed by Cundall and Strack [1], the torque is caused by tangential forces $\mathbf{F}^t_{kl}$.

Besides the tangential force, contribution of rolling may be remarkable. Rolling was defined as relative angular rotation of two contacting bodies about an axis parallel to their common tangent plane without sliding. Various approaches to this problem have been elucidated in theoretical and numerical studies [8,20–27].

The rolling torque T^{roll}_{kl} is defined on the basis of [22–24] and reflects rolling resistance defined prior to rolling by the elastic component $T^{roll,el}_{kl}$ and during rolling by $T^{roll,fric}_{kl}$ as

$$T^{roll}_{kl} = \min\left(T^{roll,el}_{kl}, T^{roll,fric}_{kl}\right), \tag{1}$$

The decisive role belongs to frictional component, calculated for the contacting spheres k and l as follows:

$$T^{roll,fric}_{kl} = -f\ \min\left(R_k, R_l\right)\ |\mathbf{F}^n_{kl}|, \tag{2}$$

where $\mathbf{F}^n_{kl}$ is the normal contact force, R_k and R_l are the radii of the contacting spheres. The rolling torque is independent of the angular velocity, while f is nondimensional coefficient. The developed 3D multi-sphere particle was implemented into the original parallel code DEMMAT [28].

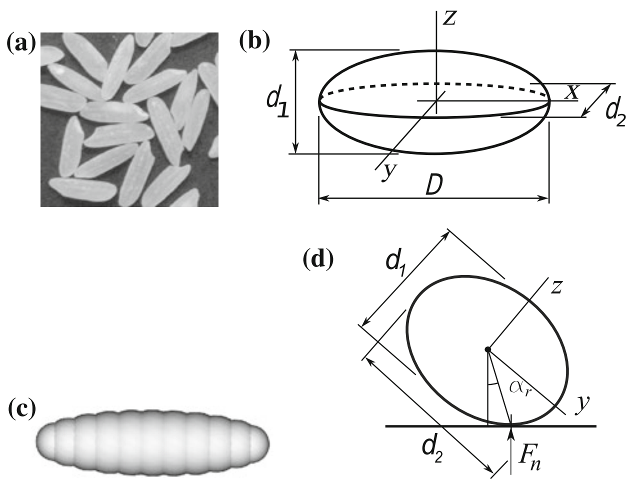

Fig. 1 The geometry of rice grains (**a**), measured diameters (**b**), the constructed multi-sphere model (**c**) and a sketch of the particles cross-section (**d**)

3 Problem description

Theoretical models require thorough examination by numerical simulation on both macroscopic and particle scale. It should be noted that the flow of particles in hoppers and piling have been considered for many years to be important benchmark tests for studying new research techniques for granular simulations. For the above reasons, the performance of 3D MS models and their suitability for simulation of rice grain flow were studied by considering the formation of the pile via hopper discharge.

3.1 A description of material

Granular material composed of long-grain milled rice grains was considered. The geometry of the particle is extracted by measuring real grains (Fig. 1a). Three principle sizes, d_1, d_2 and D (Fig. 1b), of twenty randomly selected rice grains were measured. The average values were calculated from the data obtained. It is obvious that rice grains are non axi-symmetrical particles, consequently, $d_1 \neq d_2$. Therefore, in order to fit axial symmetry required for particles model, the average value of $d = d_{ave} = (d_1 + d_2)/2$ equal to 1.93 mm was obtained. The largest size of particle D ranged from 6.2 to 7.3 mm, while the average value $D_{ave} = 6.75\,mm$ was obtained on the basis of measurements. Using the above data, the average aspects ratio $s = D_{ave}/d_{ave} = 3.5$ was defined. Finally, a set of particles with randomly defined sizes of D and fixed aspects ratio $s = 3.5$ was generated. The values of D are uniformly distributed in the range from 6.2 mm to 7.3 mm. On the basis of numerical experiments [11], the final particle model was composed by 11 spheres (Fig. 1c).

The proper choice of the grains physical properties is a difficult task, therefore, some values were taken from the available references [29,30] or simply assumed and kept constant during the simulation. The density of the particles material was calculated based on the mass of the rice grains used in the experiment, which was divided by the volume of particles used in the numerical analysis. It was obtained to be equal to 1,574 kg/m^3. Young's modulus of rice grains $E = 200$ MPa, corresponding to 19 % of moisture content (according to Zhang et al. [30]), was used in the numerical analysis, while Poisson's ratio was assumed to be $\nu = 0.2$ [29]. The tangential friction coefficient for contacts between the rice particle and Plexiglas wall was set to 0.2. The restitution coefficient was selected to be equal to 0.5.

The coefficient f in (2) is interpreted from the particle geometry (Fig. 1d) by

$$f = \tan \alpha_r. \qquad (3)$$

Finally, the approximate value $f = 0.3$ was obtained from the measured rice particle cross section.

3.2 Experimental setup

A small plane wedge-shaped hopper model made from Plexiglas with the rectangular orifice was used for investigation purposes. The depth of the hopper of 21 mm was equal approximately to eleven minor sizes of the particle. The size of a horizontal orifice was 15 × 21 mm. The half angle of the hopper was approximately equal to 25°. The hopper was positioned above the horizontal plane at the height of 68 mm.

The rice grains were poured in the hopper from a box and distributed within the hopper, forming a convex surface. The top surface height above the orifice was about 95–105 mm. Based on the material volume, $V_M = 133\,\text{cm}^3$, the average density of 790 kg/m^3 was calculated. The particles were centrally discharged by opening the orifice. They flowed slowly, falling on the smooth plane, forming a pile. The discharge time between the opening of the orifice until the last particle left in the hopper was fixed and the repose angle was evaluated by measuring the final shape of the conical pile. The experiment had been repeated 5 times to eliminate random influences.

3.3 Numerical simulation

A composition of $N = 5000$ particles, whose properties are described above, was used in DEM simulations. The MS model presented is implemented to mimic the experiment conditions on the natural scale.

The simulation was performed in two stages. At the first stage of analysis, the elongated particles were generated at random positions and orientation in a cubic volume above the hopper without the overlap between the particles. The gravity acceleration (9.81 m/s^2), causing the particles to fall down to the bottom of the hopper, was applied. The constant time step $\Delta t = 10^{-6}$ s was selected, which was about 100 times shorter than the time of collision between the particle and the wall. The numerically obtained average material density of 818 kg/m^3 is comparable with the experimental value of 790 kg/m^3.

At the second stage, the discharge of the hopper was simulated. The particles fall down under the action of gravity on the bottom plane, forming a conical pile. The simulation was interrupted, when $t = 3$ s, which is sufficient to reach zero kinetic energy of the particle system. Every numerical experiment with specified parameters had been repeated 3 times, thereby applying randomly generated initial particle sizes and positions.

4 Results and discussion

A series of numerical experiments was conducted to investigate the influence of friction. A prescribed set of values of tangential friction coefficient μ, ranging between 0.1 and 1.0, were applied to study the sensitivity of piling to tangential friction and to fit the experiment. The conventional DEM methodology neglecting rolling resistance with zero rolling friction coefficient, $f = 0$, was considered in the first case.

Simulation results in terms of the average repose angle of the pile (Fig. 2a) and the average discharge time (Fig. 2b) are shown by dash-dot curves, while scattering of the values is also indicated graphically. Here, experimentally measured average values along the uncertainty margins are shown for the sake of comparison.

The results obtained illustrate the inconsistency of this modelling approach because the obtained values for the repose angle lie below the experimental results.

The second series of numerical experiments was conducted by DEM, considering rolling resistance. The presence of rolling friction is expected to be a required attribute of the MS model developed. The value of coefficient $f = 0.3$ calculated based on the geometry of the rice grain and described in Sect. 3 was used.

The newly obtained results are presented in Fig. 2 by solid curves. The resulting curves show that the best agreement with both experimental values could be reached by using tangential friction coefficient of about 0.425.

As follows from the simulation, the influence of rolling may be roughly evaluated by comparing the differences between the provided experimental and DEM model data without introducing rolling resistance ($f = 0$).

To clarify the role of rolling resistance, a comprehensive analysis was performed. The geometry of the flowing material is probably the simplest adequacy criterion. A snapshot of the discharged material after 1.0 s is presented in Fig. 3, while the final views of piles are shown in Fig. 4. Here, the experimental results are compared with two cases of simulation. The numerical results present the view of the central section. Each of the ten colours marks a portion of 500 particles which sequentially flow through the orifice, thereby indicating their mobility during discharge and when forming a pile.

Qualitatively, the pictures are quite similar, however, some remarkable differences may be found. The numerical model with rolling friction better responds to the experimentally observed character of the pile shape, while the numerical model without rolling friction indicates higher mobility of particles resulting in a more flat pile compared to the experiment.

The obtained numerical results gave us a possibility to extract more details and parameters. The main effects may be attributed to the rotational motion, quantitatively reflected by time histories of the kinetic energy. The rotational kinetic energy of the particle systems presents the sum of energies of individual particles. The kinetic energy of each symmetrical particle may be composed of energies of three independent local rotations in terms of the moment of inertia and the rotation angle. For elongated particle it is presented by two components, $E_{r,sym}$ and $E_{r,non-sym}$, considering local rotations about the axis of symmetry and the two remaining

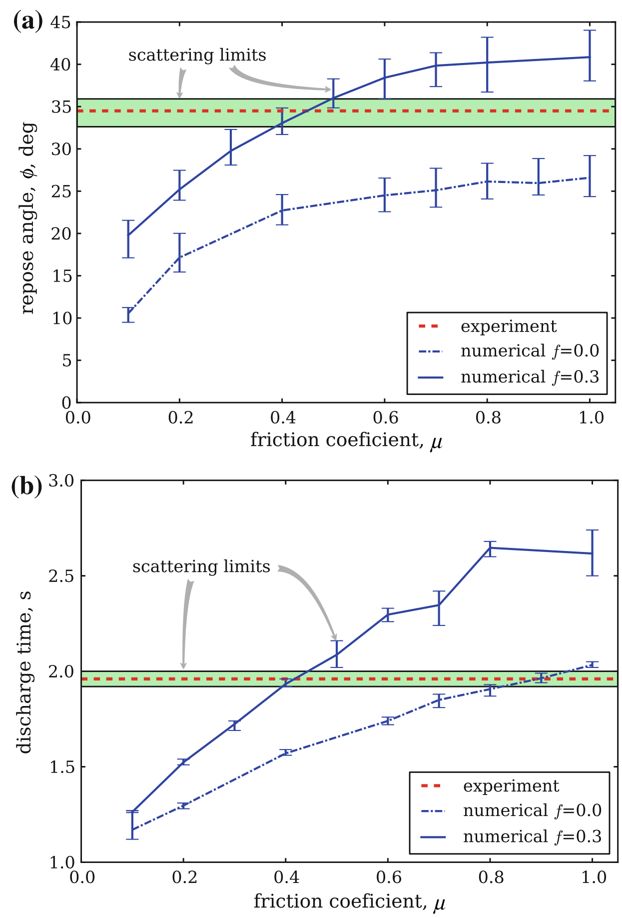

Fig. 2 Variation of granular parameters versus tangential friction: **a** repose angle of the pile, **b** discharge time

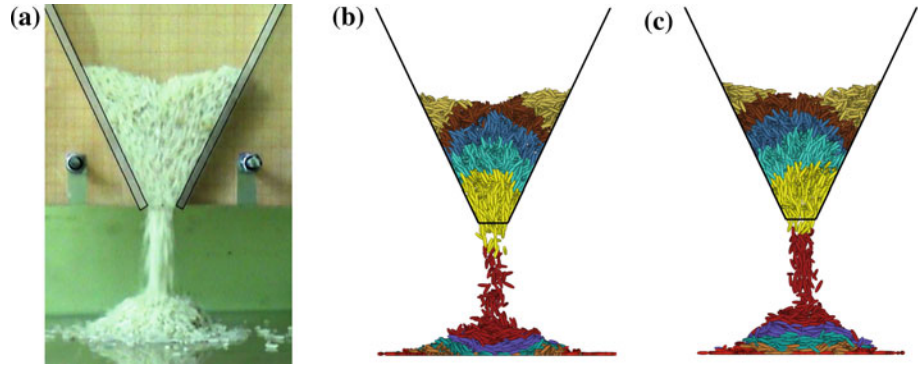

Fig. 3 A snapshot of the particle flow during the discharge: an experimental view (**a**), numerical results of the DEM without introducing rolling friction (**b**) and with rolling friction (**c**)

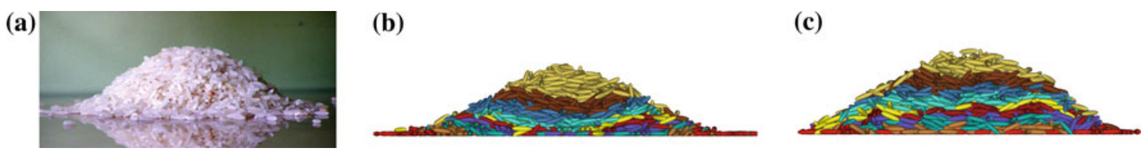

Fig. 4 A view of the formed piles: experimental view (**a**), numerical results of DEM without introducing rolling friction (**b**) and DEM with rolling friction (**c**)

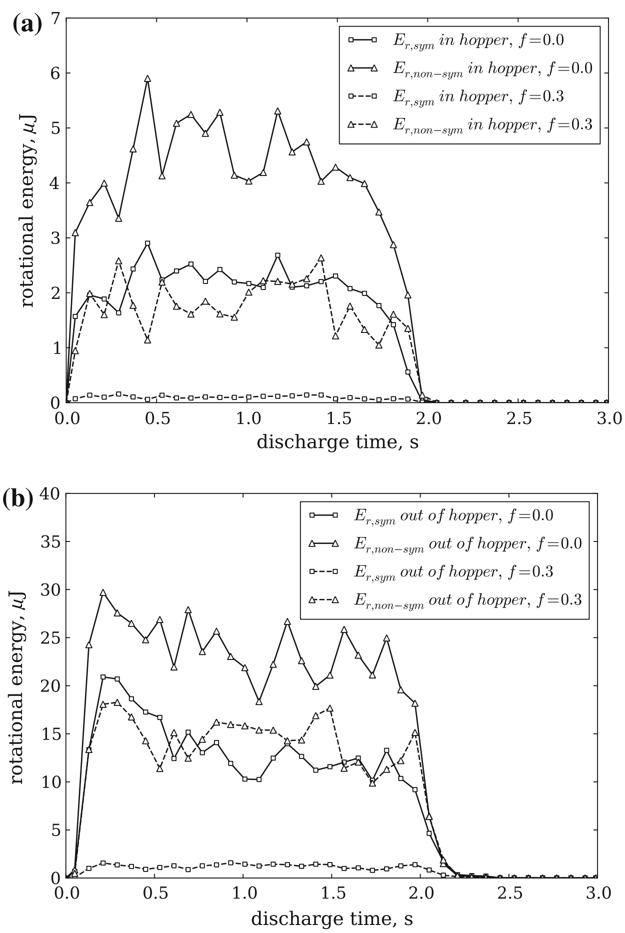

Fig. 5 Time histories of the rotational energy in the hopper (**a**) and out of the hopper (**b**)

perpendicular axes, respectively. The rotational energy of particles inside the hopper are presented in Fig. 5a, while the energies of particles streaming from the hopper and forming the pile are shown in Fig. 5b. To avoid strong fluctuations all graphs are presented by reduced number of averaged values.

Here, rolling friction practically suppresses local spin, while the perpendicular rotation occurs because of the collective particles rearrangement. It is clearly shown that rolling effects are remarkable for rotational behaviour. The graph confirms the previous observations that neglecting of this rolling friction effect leads to overincreased capability of particles to rotate by falling on the pile.

5 Conclusions

The capability of the axi-symmetric multi-sphere (MS) to model the elongated irregular shaped particles was examined. Based on the simulation results and experimental validation, it can be generally stated that axi-symmetric MS approach is capable of modelling friction effects of the elongated particles of irregular shape, however, rolling interaction must be taken into account. The particular observations arising from this study can be summarised in the following manner.

Computational results provide quantitative evidence about the increase of rolling friction due to geometric deviations of the particles shape from the axi-symmetrical geometry. Thus, geometric evaluation of rolling may be reasonable, while neglecting of rolling resistance of an elongated non-symmetrical particle leads to artificial increase of local rotations.

The validation of the tangential and rolling friction coefficients by the discharge time and repose angle of the pile confirmed that macroscopic parameters reflect the combined effect of grain scale parameters. It was demonstrated that separate validations of the tangential friction coefficient by various macroscopic parameters (e.g. the discharge time or repose angle, in our case) can yield different results. Consequently, the validation based on a larger number of parameters is preferable. A more systematic study of all model parameters should be made in the future.

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References

1. Cundall, P.A., Strack, O.D.L.: A discrete numerical model for granular assemblies. Geotechnique **29**, 47–65 (1979)
2. Džiugys, A., Peters, B.J.: An approach to simulate the motion of spherical and non-spherical fuel particles in combustion chambers. Granul. Mater. **3**, 231–266 (2000)
3. Wellmann, C., Lillie, C., Wriggers, P.: A contact detection algorithm for superellipsoids based on the common-normal concept. Eng. Comput. **25**, 432–442 (2008)
4. Pena, A., Garcia-Rojo, R., Herrmann, H.J.: Influence of particle shape on sheared dense granular media. Granul. Matter **9**, 279–291 (2007)
5. Pournin, L., Weber, M., Tsukahara, M., Ferrez, J.-A., Ramaioli, M., Liebling, T.M.: Three-dimensional distinct element simulation of spherocylinder crystallization. Granul. Matter **7**(23), 119–126 (2005)
6. Favier, J.F., Abbaspour-Fard, M.H., Kremmer, M., Raji, A.O.: Shape representation of axisymmetrical, non-spherical particles in discrete element simulation using multielement model particles. Eng. Comput. **16**, 467–480 (1999)
7. Abbaspour-Fard, M.H.: Theoretical validation of a multi-sphere, discrete element model suitable for biomaterials handling simulation. Biosyst. Eng. **88**, 153–161 (2004)
8. Zhou, C., Ooi, J.Y.: Numerical investigation of progressive development of granular pile with spherical and non-spherical particles. J. Mech. Mater. **41**(6), 707–714 (2009)
9. Khanal, M., Raghuramakrishnan, R., Tomas, J.: Discrete element method simulation of effect of aggregate shape on fragmentation of particle composites. Chem. Eng. Technol. **31**(10), 1526–1531 (2008)
10. Kruggel-Emden, H., Rickelt, S., Wirtz, S., Scherer, V.: A study on the validity of the multi-sphere discrete element method. Powder Technol. **188**(2), 153–165 (2008)
11. Markauskas, D., Kačianauskas, R., Džiugys, A., Navakas, R.: Investigation of adequacy of multi-sphere approximation of elliptical particles for DEM simulations. Granul. Matter **12**(1), 107–123 (2010)
12. Härtl, J., Ooi, J.Y.: Experiments and simulations of direct shear tests: porosity, contact friction and bulk friction. Granul. Matter J. (Special Issue) **10**, 263–271 (2008)
13. Coetzee, C.J., Els, D.N.J.: Calibration of discrete element parameters and the modelling of silo discharge and bucket filling. Comput. Electron. Agric. **65**(2), 198–212 (2009)
14. Raji, A.O., Favier, J.F.: Model for the deformation in agricultural and food particulate materials under bulk compressive loading using discrete element method. I: Theory, model development and validation. J. Food Eng. **64**, 359–371 (2004)
15. Sakaguchi, E., Suzuki, M., Favier, J.F., Kawakami, S.: Numerical simulation of the shaking separation of paddy and brown rice using the discrete element method. J. Agric. Eng. Res. **79**(3), 307–315 (2001)
16. Alonso-Marroquin, F., Wang, Y.: An efficient algorithm for granular dynamics simulations with complex-shaped objects. Granul. Matter **11**, 317–329 (2009)
17. Tsuji, Y., Tanaka, T., Ishida, T.: Lagrangian numerical simulation of plug of cohesionless particles in a horizontal pipe. Powder Technol. **71**, 239–250 (1992)
18. Balevičius, R., Džiugys, A., Kačianauskas, R., Maknickas, A., Vislavičius, K.: Investigation of performance of programming approaches and languages used for numerical simulation of granular material by the discrete element method. Comput. Phys. Comm. **175**, 404–415 (2006)
19. Balevičius, R., Kačianauskas, R., Mroz, Z., Sielamowicz, I.: Discrete-particle investigation of friction effect in filling and unsteady/steady discharge in three-dimensional wedge-shaped hopper. Powder Technol. **187**, 159–174 (2008)
20. Zhou, Y., Yang, R.Y., Yu, A.B.: Discrete particle simulation of particulate systems: theoretical developments. Chem. Eng. Sci. **62**, 3378–3392 (2007)
21. Luding, S.: Cohesive, frictional powders: contact models for tension. Granul. Matter **10**, 235–246 (2008)
22. Zhou, Y.C., Wright, B.D., Yang, R.Y., Xu, B.H., Yu, A.B.: Rolling friction in the dynamic simulation of sandpile formation. Phys. A **269**, 536–553 (1999)
23. Iwashita, K., Oda, M.: Micro-deformation mechanism of shear banding process based on modified distinct element method. Powder Technol. **109**, 192–205 (2000)
24. Tordesillas, A., Walsh, D.C.S.: Incorporating rolling resistance and contact anisotropy in micromechanical models of granular media. Powder Technol. **124**(1-2), 106–111 (2002)
25. Zhu, H.P., Yu, A.B.: Steady-state granular flow in a three-dimensional cylindrical hopper with flat bottom: microscopic analysis. J. Phys. D Appl. Phys. **37**, 1497–1508 (2004)
26. Jiang, M.J., Yu, H.-S., Harris, D.: A novel discrete model for granular material incorporating rolling resistance. Comput. Geotech. **32**(5), 340–357 (2005)
27. Markauskas, D., Kačianauskas, R.: Investigation of the rolling resistance in DEM simulations of piling. J. Vibroeng. **11**(3), 482–490 (2009)
28. Kačianauskas, R., Maknickas, A., Kačeniauskas, A., Markauskas, D., Balevičius, R.: Parallel discrete element simulation of poly-dispersed granular material. Adv. Eng. Softw. **41**, 52–63 (2010)
29. Shitanda, D., Nishiyama, Y., Koide, S.: Compressive strength properties of rough rice considering variation of contact area. J. Food Eng. **53**, 53–58 (2002)
30. Zhang, Q., Yang, W., Sun, Z.: Mechanical properties of sound and fissured rice kernels and their implications for rice breakage. J. Food Eng. **68**, 65–72 (2005)