VI International Conference on Particle-based Methods – Fundamentals and Applications
PARTICLES 2019
E. Oñate, M. Bischoff, D.R.J. Owen P. Wriggers, , & T. Zohdi (Eds)

MICROSCOPIC CALIBRATION OF ROLLING FRICTION TO MIMIC PARTICLE SHAPE EFFECTS IN DEM

RICCARDO RORATO[1], MARCOS ARROYO[2], ANTONIO GENS[3] AND EDWARD ANDÒ[4]

[1] Universitat Politècnica de Catalunya (UPC)
Department of Civil and Environmental Engineering, 08034 Barcelona (Spain)
riccardo.rorato@upc.edu

[2] Universitat Politècnica de Catalunya (UPC)
Department of Civil and Environmental Engineering, 08034 Barcelona (Spain)
marcos.arroyo@upc.edu

[3] Universitat Politècnica de Catalunya (UPC)
Department of Civil and Environmental Engineering, 08034 Barcelona (Spain)
antonio.gens@upc.edu

[4] Université Grenoble Alpes, CNRS
Grenoble INP, 3SR, F-38000 Grenoble (France)
edward.ando@3sr-grenoble.fr

Key words: Granular Materials, DEM, Particle Shape, Rolling Resistance, Contact Problems.

Summary. *It is widely recognised that particle shape influences the mechanical response of granular materials [1-2]. Rolling resistance elasto-plastic contact models are frequently used to approximate particle shape effects in simulations using the Discrete Element Method (DEM) [3-4]. Such contact models require calibration of several micro-parameters, most importantly a rolling resistance coefficient. In this work, the rolling resistance has been calibrated to reproduce the triaxial tests – in terms of mechanical and kinematic responses – of two different sands: Hostun and Caicos sands. The value of rolling resistance is directly linked to true sphericity, a basic measure of grain shape, as originally proposed in Rorato et al. (2018) [5]. When shape measurements are performed* [6]*, this link enables independent evaluation of the rolling resistance coefficient for each particle. It does also allow the characteristic shape variability of natural soils to be easily taken into account.*

1 INTRODUCTION

Much work has been done to characterise granular shape and to understand its influence on overall soil behavior. Thus, Wadell (1932) [7] introduced the concept of “sphericity” that quantifies how a particle differs from a sphere, in terms of surface area. Krumbein (1941) [8] presents the first chart to visually estimate shape from the grain lengths ratios.

There is much evidence showing that particle shape is relevant for mechanical responses of soils. Andò (2013, 2012) [1], [9] tested in triaxial conditions different sands with shape ranging from very angular to rounded. Using Digital Image Correlation, he showed that angular sands exhibited a larger shear band thickness compared to rounded sands. Rorato *et al.* (2019) [10] demonstrated that a rounded sand (Caicos ooids) exhibits higher grains rotations compared to an angular sand (Hostun sand).

In this work, we propose a new procedure for an optimal calibration of the DEM contact model parameters that is able to mimic the effect of particle shape without dramatically increase the computational time. In particular, our approach aims to (1) limit the number of free parameters requested, (2) respect the mechanical and kinematic triaxial responses of the sheared granular materials and (3) maintain low the computational time. The Particle Flow Code (PFC5) developed by Itasca Inc. has been used.

2 DESIGN AND ANALYSIS

The most widely used shape used in DEM is the sphere, because it allows straightforward and computationally efficient contact detection. Unfortunately, soil particles are not spheres. Some researchers has tried to tackle this challenge by introducing *non-spherical* elements, like clumps (*e.g.,* [11], [12]), polyhedrons (*e.g.,* [13], [14]) or grain-shape-inspired particles (*e.g.*, [15], [16]), at the price of increasing dramatically the complexity of the contact detection and computational time. Other researchers (*e.g.*, [3], [4], [17]) have proposed the introduction of a resisting moment (*i.e.*, rolling resistance) into the contact law, beside normal and shear forces, in order to consider the influence of flat (*i.e.,* not punctual) contacts between real grains.

In this work, a simplified version - as implemented in the PFC5 software - of the Iwashita & Oda contact model [3] has been used under the following assumptions:
(1) The *rolling stiffness* (k_r) is defined as the Iwashita & Oda's original contact model:

$$k_r = k_s R_r^{\ 2} \tag{1}$$

where k_s is the contact *shear stiffness* and R_r the *effective radius* defined as

$$R_r = \frac{1}{R_1} + \frac{1}{R_2} \tag{2}$$

being R_1 and R_2 the radii of the two particles in contact.
(2) The moment-rotational contact law is implemented as an elastic-perfectly plastic model with the yielding moment (M^*) defined as:

$$M^* = \mu_r F_n R_r \tag{3}$$

where μ_r is defined as *rolling friction coefficient* and F_n is the normal contact force.

This paper exploits a novel approach to relate the particle shape with the rolling resistance applied at the contacts, extending the model that was originally proposed in Rorato *et al.*

(2018) [5]. In particular, it is hypothesized that the *degree of true sphericity* [1](ψ), of one particle is univocally related with its *coefficient of rolling friction*, through a relation

$$\mu_r = F(\psi) = F\left(\frac{S_n}{S}\right) \tag{4}$$

valid for all the spherical particles participating in the DEM simulation. Therefore, if the statistical distribution of sphericity is known for one particular sand, it is possible to extract infinite values so that one measure of ψ can be assigned to each sphere of the numerical specimen, and therefore the *rolling friction coefficients* can distributed through all the discrete elements. The histograms of true sphericity for three different sands (Hostun, Caicos and Ticino sands), computed as in Rorato *et al.* (2019) [6], are showed in Figure 1.

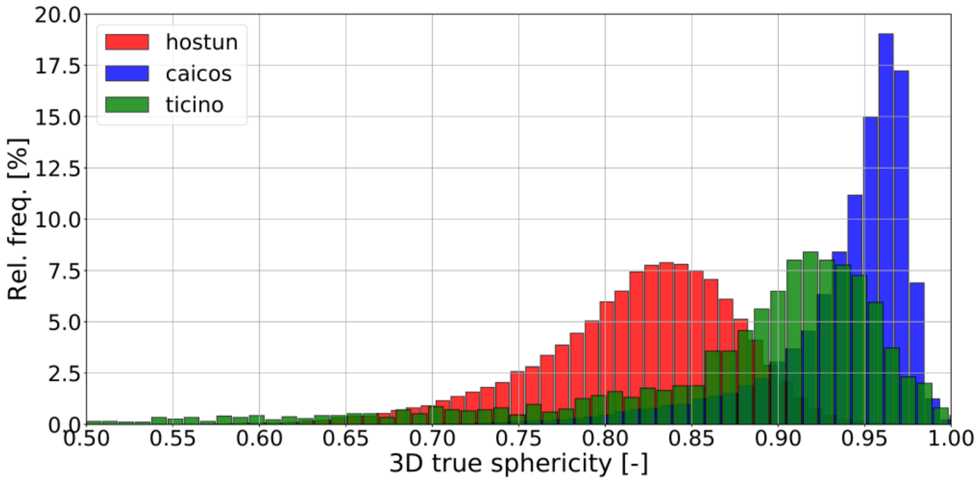

Figure 1: Statistical distributions of 3D true sphericity for Hostun, Caicos and Ticino sands.

The question then is what shape function $F(\psi)$ might take. We tried to find the equation of $F(\psi)$ that could best match the experimental triaxial tests performed on Hostun sand (specimen "HNEA01") and Caicos ooids (specimen "COEA01"). The calibration procedure here proposed aims to fit the conventional macro-mechanical responses together with kinematic measures. In particular, the histories of the cumulated grain rotations are known for each grain from the experiments have been measured and the particles rolling frictions have been adjusted to reproduce similar kinematic responses inside the shear bands of the numerical specimens. It is indeed well known from past DEM studies [18]–[21] that the same macroscopic friction angle can be obtained from several couples of *sliding friction coefficient* (μ) and *rolling friction coefficient* (μ_r). Both parameters contribute to the shear resistance of the numerical sample, and their influence is coupled. However, the rotational information - from the experimental measures of grains rotations - provides a unique numerical solution.

[1] Defined by Wadell (1932) [7] as the ratio between the surface area (S_n) of the equivalent sphere (*i.e.,* same volume as the grain) and the surface area (S) of the particle.

3 RESULTS AND DISCUSSION

The equation of $F(\psi)$ has been finally chosen, after an iterative procedure, according to a power law written as

$$\mu_r = 0.1963(\psi)^{-8.982} \tag{5}$$

with an upper bound fixed at $\psi = 1$ (perfect sphere).

This relationship allows a good fit of the macro-mechanical responses (*i.e.,* stress-volumetric-strain) of HNEA01 and COEA04 sand specimens and the mean rotations inside the shear bands (*i.e.,* the kinematics at failure) throughout the execution of the triaxial test.

Particles belonging to the shear bands, in both the physical and numerical specimens, have been identified according to a procedure originally proposed by Catalano [22] and detailed in Rorato *et al.* (2019) [10] for the two sand considered in this study.

The proposed approach has been then tested for validation in three different situations, achieving successful results, (1) at higher confining pressures, (2) testing a third type of sand (Ottawa sand) for which the statistical distribution of 3D sphericity was known and (3) testing a fourth type of sand (Ticino sand) for which the distribution of 3D sphericity was not known. Regarding the third case, an innovative method is exploited to determine the statistical distribution of the *degree of true sphericity* (3D shape parameter) from 2D measures, as originally proposed by Rorato *et al.* (2019) [6]. In particular, a table scanner has been used to obtain an "oriented" projection of thousands of sand grains laying on their *plane of greatest stability*. The 2D outlines of all the particles thus obtained, can be then studies by image analysis techniques in order to extrapolate[2] the statistical distribution of ψ, and therefore of μ_r, according to Eq. 5.

The values of rolling frictions obtained from Eq. (5) have been compared to the ones computed using a completely different -geometrical- approach originally proposed by Wensrich & Katterfeld (2012) [20] and then improved in [21]. In particular, they claimed that rolling resistance is originated at the micro-scale level by the eccentricity of the contact, as shown in Figure 3.

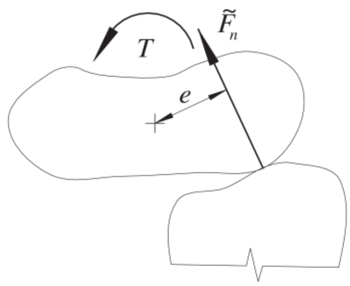

Figure 3: Contact of un-spherical particles producing a torque (*T*) due to the eccentricity (*e*) of the normal contact force (F_n) [20]

[2] It is known from [6] that the degree of true sphericity (ψ) is highly correlated with the *perimeter sphericity*, 2D shape parameter, after "oriented" particle projection (*i.e.,* perpendicularly to the minor particle length).

Assuming the magnitude of the torque T at the contact equal to

$$|T| = e|F_n|$$

and being M^* the limiting value of from the contact model (Eq. 3), Wensrich & Katterfeld supposed that a good estimation of the rolling friction is obtained imposing $|T| = M^*$, that leads to

$$\mu_r = \frac{\langle e \rangle}{R_r}$$

where $\langle e \rangle$ is the average eccentricity of contact over all possible contacts and R_r is the rolling radius.

In this work, we compute the values of μ_r using this approach for all the grains of HNEA01 and COEA04, and we compare them with the values obtained from Eq. 5. The average eccentricity and the rolling radius of each grain are computed numerically exploiting the vertices of the surface mesh created by the Marching Cubes algorithm implemented in the Scikit-image python library [23]. The comparison between the two approaches is shown in Figure 4.

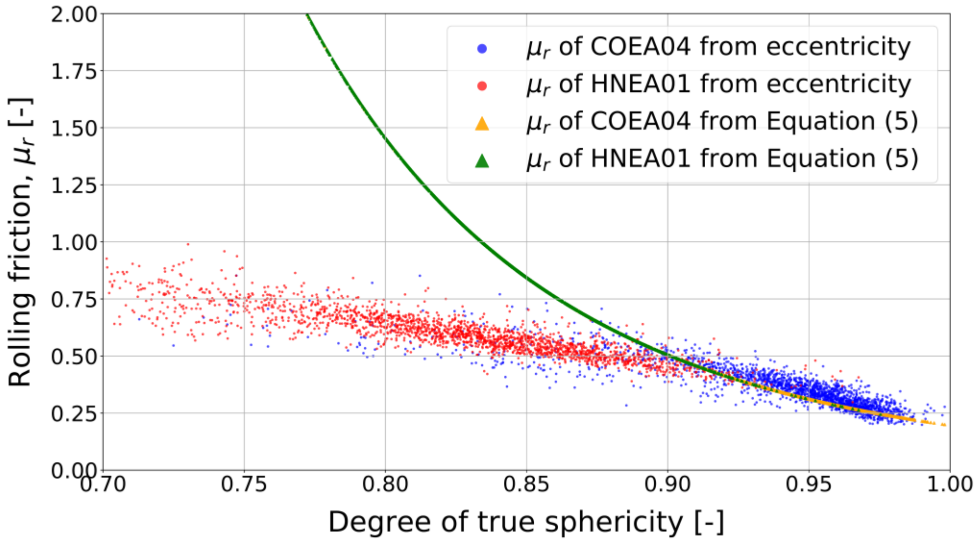

Figure 4: Rolling frictions of all particles involved in the simulation obtained from both eccentricity calculation and Equation 5. For high values of particle sphericity (*i.e.*, ψ>0.90) the two approaches provide similar values.

It is evident from Figure 4 that both approaches provide values of rolling frictions that decrease with particle sphericity, as expected. It is somehow surprising that the two approaches, although conceptually completely different, provide similar rolling frictions values, especially at higher values of particle sphericity (*i.e.*, ψ>0.90). Both approaches suggest that even for very spherical grains, a coefficient of rolling friction of about 0.20 should be assigned. However, the results start diverging when the grains become more angular. It worth reminding that Eq. (5) has been design to match the experimental material responses. Therefore, if the rolling frictions from the eccentricity calculations were assigned in the DEM simulation, the numerical response would be weaker compared to the experiments, especially for specimen HNEA01. It means that the geometrical description of particle shape is not sufficient to capture all of the contributions provided by shape to the shearing material resistance. However, some other contributions (*e.g.,* grain interlocking, adhesion), which are not directly related to shape as a geometric property of one single particle, are somehow included in the proposed relationship described by Eq. (5).

4 CONCLUSIONS

This paper presents an innovative technique to relate univocally the degree of true sphericity of each grain contained in a sand sample with the coefficient of rolling friction to apply to its numerical avatar of spherical shape. The main advantage of the proposed model is that it reduces the number of free parameters to set by trial-and-error procedures when performing DEM simulations, albeit respecting the grains kinematics at failure. Indeed, if the statistical distribution of sphericity is known, either from experiments either from the literature, the resisting rolling moment is entirely determined since all the parameters involved in the contact model are known or predictable.

The contact detection remains economical and advanced algorithms are not required, maintaining low the computational time. This will open new frontiers to the use DEM for studying engineering applications at larger scales, especially in geotechnical problems in which the particulate nature of the soil cannot be ignored.

5 REFERENCES

[1] E. Andò, "Experimental investigation of microstructural changes in deforming granular media using x-ray tomography," PhD Thesis. Université de Grenoble, 2013.

[2] J. Santamarina and G. Cho, "Soil behaviour: The role of particle shape," in *Advances in Geotechnical Engineering. Proceedings of the Skempton Conference*, 2004, pp. 1–14.

[3] K. Iwashita and M. Oda, "Rolling resistance at contacts in simulation of shear band development by DEM," *J. Eng. Mech.*, vol. 124, no. 3, pp. 285–292, 1998.

[4] M. J. J. Jiang, H.-S. Yu, and D. Harris, "A novel discrete model for granular material incorporating rolling resistance," *Comput. Geotech.*, vol. 32, no. 5, pp. 340–357, 2005.

[5] R. Rorato, M. Arroyo, A. Gens, E. Andò, and G. Viggiani, "Particle shape distribution effects on the triaxial response of sands: a DEM study," in *micro to MACRO Mathematical Modelling in Soil Mechanics, Trends in Mathematics*, 2018, pp. 277–286.

[6] R. Rorato, M. Arroyo, E. Andò, and A. Gens, "Sphericity measures of sand grains," *Eng. Geol.*, vol. 254, no. April, pp. 43–53, 2019.

[7] H. Wadell, "Volume, Shape, and Roundness of Rock Particles," *J. Geol.*, vol. 40, no. 5, pp. 443–451, 1932.

[8] W. C. Krumbein, "Measurement and Geological significance of shape and roundness of sedimentary particles," *J. Sediment. Petrol.*, vol. 11, no. 2, pp. 64–72, 1941.

[9] E. Andò, S. A. Hall, G. Viggiani, J. Desrues, and P. Bésuelle, "Grain-scale experimental investigation of localised deformation in sand: A discrete particle tracking approach," *Acta Geotech.*, vol. 7, no. 1, pp. 1–13, 2012.

[10] R. Rorato, M. Arroyo, E. Andò, A. Gens, and G. Viggiani, "Linking shape and rotation of grains during triaxial compression of sand," *Geotechnique*, p. (submitted), 2019.

[11] J. Katagiri, T. Matsushima, Y. Yamada, J. Katagiri, T. Matsushima, and Y. Yamada, "Simple shear simulation of 3D irregularly-shaped particles by image-based DEM," *Granul. Matter*, vol. 12, pp. 491–497, 2010.
[12] M. Lu and G. R. McDowell, "The importance of modelling ballast particle shape in the discrete element method," *Granul. Matter*, vol. 9, no. 1–2, pp. 69–80, 2007.
[13] J. Elias, "DEM simulation of railway ballast using polyhedral elemental shapes," in *PARTICLES 2013 - III International Conference on Particle-based Methods – Fundamentals and Applications*, 2013, pp. 1–10.
[14] P. Langston, J. Ai, and H.-S. Yu, "Simple shear in 3D DEM polyhedral particles and in a simplified 2D continuum model," *Granul. Matter*, vol. 15, pp. 595–606, 2013.
[15] A. X. Jerves, R. Y. Kawamoto, and J. E. Andrade, "Effects of grain morphology on critical state: A computational analysis," *Acta Geotech.*, vol. 11, no. 3, pp. 493–503, 2016.
[16] R. Kawamoto, E. Andò, G. Viggiani, and J. E. Andrade, "All you need is shape: Predicting shear banding in sand with LS-DEM," *J. Mech. Phys. Solids*, vol. 111, pp. 375–392, 2018.
[17] H. Sakaguchi, E. Ozaki, and T. Igarashi, "Plugging of the Flow of Granular Materials during the Discharge from a Silo," *Int. J. Mod. Phys. B*, vol. 7, no. 09–10, pp. 1949–1963, 1993.
[18] N. Estrada, A. Taboada, and F. Radjaï, "Shear strength and force transmission in granular media with rolling resistance," *Phys. Rev. E*, vol. 78, no. 2, pp. 1–11, 2008.
[19] K. Cheng, Y. Wang, Q. Yang, Y. Mo, and Y. Guo, "Determination of microscopic parameters of quartz sand through tri-axial test using the discrete element method," *Comput. Geotech.*, vol. 92, pp. 22–40, 2017.
[20] C. M. Wensrich and A. Katterfeld, "Rolling friction as a technique for modelling particle shape in DEM," *Powder Technol.*, vol. 217, pp. 409–417, 2012.
[21] C. M. Wensrich, A. Katterfeld, and D. Sugo, "Characterisation of the effects of particle shape using a normalised contact eccentricity," *Granul. Matter*, vol. 16, no. 3, pp. 327–337, 2014.
[22] E. Catalano, B. Chareyre, and E. Barthélémy, "Pore-scale modeling of fluid-particles interaction and emerging poromechanical effects," *Int. J. Numer. Anal. Methods Geomech.*, vol. 38, no. 1, pp. 51–71, Jan. 2014.
[23] S. van der Walt *et al.*, "scikit-image: image processing in Python," *PeerJ*, vol. 2:e453, 2014.