Investigation of multi-sphere models in DEM simulations of granular flow - comparison with smooth ellipsoids

Rimantas Kačianauskas[1], **Darius Markauskas**[1], **Algis Džiugys**[2] and **Robertas Navakas**[2]

[1]*Laboratory of Numerical Modelling, Vilnius Gediminas Technical University, Saulėtekio al. 11, LT-10223 Vilnius, Lithuania*
e-mail: rkac@vgtu.lt; darius markauskas@vgtu.lt

[2]*Laboratory of Combustion, Lithuanian Energy Institute, Breslaujos g. 3, LT-44403 Kaunas, Lithuania*
e-mail: dziugys@isag.lei.lt; rnavakas@mail.lei.lt

Abstract

Simulation of dry non-cohesive visco-elastic granular materials by the Discrete Element Method (DEM) is considered. This work addresses the problem of particle shape. The Multi-Sphere (MS) approach to approximation of the smooth ellipsoidal particle with the increasing number of sub-spheres is studied by solving a piling problem and qualitative and quantitative comparison of both models is presented. Based on the simulation results obtained, it could be stated that MS model approximates the smooth particle within the limits of the appropriate tolerance. A macroscopic MS model possesses, however, different interaction behaviour of particles on microscopic level. It has been demonstrated how artificial increase of the friction coefficient is related to the number of sub-spheres.

Keywords: granular material, discrete element method, particle shape, multi-spheres, porosity, friction

1. Introduction

Numerical simulations present a reliable tool for investigating of particulate materials in many areas. The Discrete Element Method (DEM) is the most suitable numerical approach to capture the discrete nature of particle system by a discrete set of quantities. Because of large number of particles, simple analytical inter-particle contact models are employed to reduce computational expenses. It is rather simple task for spheres, but handling of other shapes makes problem much more complicated.

Elliptical particles (ellipses and 3D ellipsoids) are probably the most widely used regular non-spherical shapes because various particles of granular material resemble these shapes. Analytical methods of contact for two- and three-dimensional elliptical particles were considered in [1].

Representation of the particle shape by the *multi-sphere* (MS) approach appears to be a promising alternative. Contact detection efficiency and simplicity of implementation, using sphere-to-sphere contact, is the main advantage of the multi-sphere model. A general approach for representation of axi-symmetrical non-spherical particles by rigidly connected multi-spheres is suggested by Favier et al. [2].

Various details and frictional behaviour of MS applications were investigated by Pöschel and Buchholtz [3]. The approximation of sphere by MS model was considered by Kruggel-Emden et al. [4]. The application of a large number spheres allows to interpret shape deviations as roughness of the smooth surface. A simple and fast original method to create irregular particle shapes for the discrete element method using overlapping spheres is described by Ferellec and McDowell [5].

This work addresses the application of the multi-sphere approach to the modelling of elliptical particles with emphasis on evaluation of artificial increase of friction coefficient due to the approximation of smooth particle surface. The performance of the multi-sphere particle model is demonstrated by solving a piling problem.

2. MS models and simulation methodology

A three-dimensional rotational ellipsoidal particle is considered to be visco-elastic body. Its MS model is composed of n sub-spheres which are rigidly fixed with respect to each other and are located on the axis of rotational symmetry. Sub-spheres are inscribed into the ellipsoid; therefore, each of them remains tangent to ellipsoidal surface. It is assumed that variable inter-sphere distances vary proportionally to ellipsoid ordinate. On this basis, the recurrent relationship between distances of the neighbouring spheres was established [6]. By increasing of n, the smooth surface may be described with desired accuracy (Figure 1).

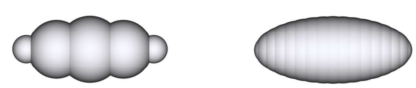

Figure 1: Geometry of multi-sphere model for ellipsoid approximated by 5 and 17 sub-spheres

The forces acting between two particles present resultant of separate contacting spheres while contact model between two spheres considers a combination of elastic, damping and friction force effects.

3. Frictional behaviour

Deviations of the MS model from the smooth surface allow artificial particles overlap. As a consequence, geometric interlocking and increased number of contacts restricts particles sliding and increases friction. Consequently, tangential friction between particles may be characterised by the effective friction coefficient μ_{eff}.

$$\mu_{eff} = \mu + \Delta\mu(n). \tag{1}$$

In the case of contact between convex smooth surfaces, μ_{eff} simply means the conventional friction coefficient μ. In the case of MS contact, the effective friction coefficient comprises additional geometric effects evaluated hereafter by Δμ

4. Numerical results

Friction effects related to MS model were investigated by conducting DEM calculations. A set consisting of 1000 mono-sized 3D ellipsoidal particles with prescribed aspect ratio $s = 2.35$ and physical properties was used for simulation purposes. Two-dimensional one side piling particles was simulated. The particles are sequentially dropped and fall down to form a pile slope. In order to capture the effect of scattering, the experiments were repeated several times while the results were presented in terms of averaged values.

The first series of numerical simulations were performed using smooth ellipsoidal particles. Thereby, a set of tangential friction coefficient μ, varying in the range from 0.2 to 1.0, was examined.

Further numerical simulations were performed using MS models of ellipsoidal particles. The number of spheres *n* varies discretely in the range from 3 to 17. MS simulations were run with the fixed value of friction coefficient $\mu = 0.3$.

The results of the MS simulations for $n = 5$ spheres are illustrated in Figure 2.

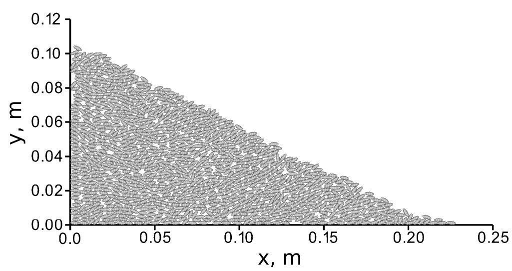

Figure 2. Simulation results of MS model ($n = 5$) -final shape of the pile with $\Phi = 26.6^{o}$

5. Discussion

Since direct measurements or numerical calculations of friction are impossible, the variation of the macroscopic parameter repose angle Φ will be used. The repose angle was obtained by evaluating the slope of the simulated pile.

The domain of the available values of repose angle $\Phi(n)$ are evaluated as follows. The upper bound of the domain $\Phi_{max} = \Phi_{MS}(n = 3) = 29.1^{o}$ is extracted from multi-sphere simulations and responds to the minimal number of spheres. The lover bound of domain Φ_0 denoted by subscript zero $\Phi_0 = \Phi_{ell} = 22.7^{o}$is extracted from the piling of smooth ellipse. This value presents convergence limit of the MS model when the number of sub-spheres *n* tends to infinity.

Finally, the effect of artificial friction was evaluated by careful examination of simulation results with the smooth ellipsoid. Therewith, limit values of friction coefficient $\mu_0 = 0.3$ and $\mu_{max} = 0.5$ are obtained. Finally, the values of the repose angle are transformed into the relationship $\Delta\mu(n)$ between friction coefficient μ and number of spheres *n*. Simulation results are presented by curve (Figure 3). Other system parameters such as porosity, coordination number, etc., may be evaluated in the same manner.

On the other hand, each of the MS models related to the number of sub-spheres *n* may be regarded as particular approximation of an ellipsoid. Deviation of the approximated shape from the perfect ellipsoid geometry may be evaluated by various characteristics, depending on the number of sub-spheres *n*. Actually, various shape factors comprising the outline, slope, area and other deviations may be employed for microscopic characterization of the MS approximation.

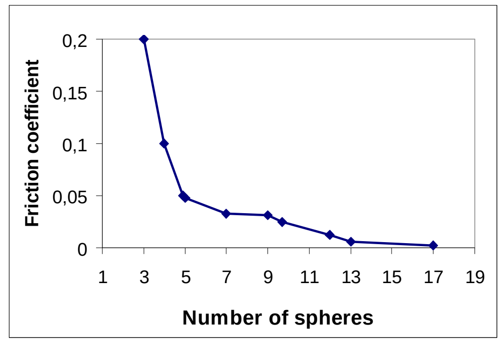

Figure 3. Variation of artificial friction coefficient against the number of sub-spheres

6. Concluding remarks

Based on the simulation results obtained, it could be stated that multi-sphere (MS) model approximates the smooth perfect ellipsoid within the limits of the appropriate tolerance**.** A macroscopic MS model possesses, however, different particles interaction on microscopic level which leads to artificial increase of friction. This effect may be evaluated numerically.

It has been found that the use of an acceptable number of sub-spheres equal to 5 (from the view point of computational efficiency) responds to increasing of dynamic friction coefficient by 0.05.

References

[1] Džiugys, A. and Peters, B.J., An Approach to Simulate the Motion of Spherical and Non-Spherical Fuel Particles in Combustion Chambers, *Granular Matter*, 3(4), pp. 231-266, 2001.

[2] Favier, J.F., Abbaspour-Fard, M.H., Kremmer, M. and Raji, A.O., Shape representation of axisymmetrical, non-spherical particles in discrete element simulation using multi-element model particles, *Engineering Computations*, 16(4), pp. 467-480, 1999.

[3] Pöschel, T. and. Buchholtz, V., Static Friction Phenomena in Granular Materials: Coulomb Law versus Particle Geometry, *Physical Review Letters*, 71(24), pp. 3963-3966, 1993.

[4] Kruggel-Emden, H., Rickelt, S., Wirtz, S. and Scherer, V.. A study on the validity of the multi-sphere Discrete Element Method, *Powder Technology*, 188(2), pp. 153-165, 2008.

[5] Ferellec, J.-F. and McDowell, G.R., A method to model realistic particle shape and inertia, *Granular Matter*, 12, pp. 459–467, 2010.

[6] Markauskas, D., Kačianauskas, R., Džiugys, A. and Navakas R., Investigation of adequacy of multi-sphere approximation of elliptical particles for DEM simulations, *Granular Matter*, 12, pp. 107-123, 2010