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Microdynamic analysis of ellipsoidal particle flow in a shear cell

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Abstract. This paper studies rheological properties of ellipsoidal particles in a model annular shear cell and compares them with the relevant parameters obtained for spherical particles under similar conditions using the discrete element method (DEM). Some important microdynamic variables such as velocity, coordination number, volume fraction and stress were considered. It was found that there are some differences between the spherical and ellipsoidal particles in terms of these properties. The feature was explained by the microscopic structures at particle scale such as those related to particle alignment and inter-particle forces.

1 INTRODUCTION

It is of paramount importance to understand the dynamical behaviour of particle flow due to the fact that it touches our daily lives from all possible directions: from residence materials like rice and sugar to commercial production facilities like pharmaceutical and food processing industry, from natural disasters like avalanches and landslides to artificial activities like transportation of pulverized coals and mixing of gravel with cement. In the earlier stages of the research field of particle flow, the primary focus was on macro-dynamic properties of the flow based on physical experiments (e,g. [1]). But it was expensive, and very much limited to detailed investigation of phenomena. The breakthrough happened with the ingenious development of numerical models.

One of the most popular methods in this area is the so-called Discrete Element Method (DEM) [2]. This method gives the best possible theoretical microdynamic description of ideal mechanical behaviour of particle conglomerate which is either stationary or in flow. The DEM has been applied in various particulate systems [3]. However, it is still far from practical function and much work is needed. Majority of earlier works using the DEM was based on spherical particles. With recent available computational resources, the research objective is inclining more in the direction of non-spherical particles due to its closeness towards practical application.

In this paper, the shear flow of ellipsoidal particles in an annular shear cell is studied, and compared with that of spherical particles under the similar conditions, in terms of some key physical properties such as particle velocity, coordination number, volume fraction and stresses. Particle alignment of the ellipsoidal particles is also examined and used to explain the difference on these properties for the non-spherical and spherical particles.

2 SIMULATION METHOD AND CONDITIONS

In this work, granular rheological analysis was performed by means of the DEM using spring dashpot model for soft particle simulation. The software package PFC3D 5.0 was utilised to simulate the flows of spherical and ellipsoidal particles in a 3D annular shear cell. The non-linear model based on Hertz-Mindlin and Deresiewicz model [4, 5] was used to calculate the contact forces between particles. The details on the DEM can be seen elsewhere [6].

A rectangular segment of widely studied annular shear cell was considered for both spherical and ellipsoidal particles (Fig. 1) here. For comparison, the cases of spherical and ellipsoidal particles have the same segment, with a dimension of 12d ×60d × h, where d is the diameter of spherical particles. The segment has two periodic boundary planes perpendicular to the x-axis. 320 spherical particles of 1.5d diameter were used to constitute each of the upper and lower platens of the segment so that the entire area of the platens was filled. The particles forming the platens possess the same physical properties (such as, density, damping coefficient, friction coefficient and stiffness) as other particles.

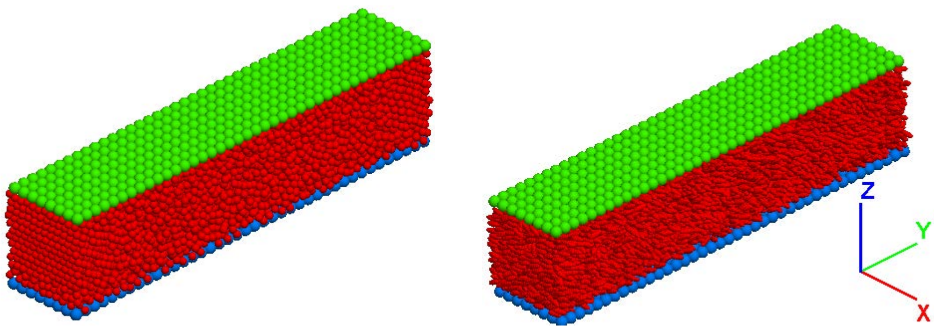

Fig. 1. Model shear cells (left: spherical, right: ellipsoidal)

The ellipsoidal particles considered have an aspect ratio of 2.5:1, and the same volume of the spherical particles. Bubble-pack algorithm [7] was used to construct these particles (Fig.2) in this work. The closed surface of the non-spherical particle was first constructed with triangular meshes of various sizes. Then spherical particles of various sizes were used to fill the space within the surface to obtain a specific volume. These particles were then glued and made immobile relative to each other and thus the particle of desired shape was constructed.

In each simulation, 10000 mono-disperse particles (spherical or ellipsoidal) are first generated randomly between the upper and lower platens with an initial volume fraction of 0.7. The position of the upper platen is then lowered gradually until the desired pressure acting on the particle assembly is applied. While the lower platen remains at the same height, the upper platen height varies to maintain the constant normal pressure. Shear rate is then gradually increased to the pre-set value after the loading has been stabilized. When the system becomes steady, the process of calculating microdynamic properties starts. The particle properties and simulation parameters are given in Table 1.

Fig. 2. Ellipsoidal particle

It is worth noting that the gravity was considered to affect the dynamic behaviours of shear flows and was ignored in some of the previous studies [8]. In this work, the gravity has been included in the simulations. Our simulations indicate that it does not have noticeable effect on granular rheology for the configurations considered. Further work will be conducted to clarify this issue.

3 RESULTS AND DISCUSSION

The results are discussed in terms of particle alignment, velocity profile, coordination number, volume fraction and stress tensor.

3.1 PARTICLE ALIGNMENT

Particle orientation (alignment) is of special interest in the study of non-spherical particles because of its strong influence on the dynamic properties of granular assembly. In this study, we observed that the ellipsoidal particles are approximately aligned with the direction of the shear velocity, as shown in Fig. 3. This means that the major axes of the particles are parallel to the flow. This finding is similar to that obtained in earlier studies (e.g., [9]). It is worth mentioning that the more elongated the particles are, the more they are aligned towards the shear flow. It has also been identified by studying the statistical distribution of the particulate inclination angles along the direction of shear velocity (not included in this paper, for brevity). The sections below will discuss on how this phenomenon affects the characteristics of flow dynamics of ellipsoidal particulate assemblies.

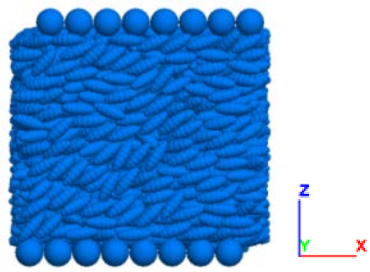

Fig. 3. Particle orientation during flow

3.2 VELOCITY PROFILE

The velocity profile was studied for assemblies of spherical and ellipsoidal particles. It was observed that being in agreement with the previous studies [8, 10], the velocity components in the y- and z-axis directions are small and can be ignored. Hence, only the velocities in the x-axis direction (direction of the flow) on the xz-plane are shown in Fig. 4.

Table 1: The particle properties and parameters used in the simulations

Property	Value	Unit
Particle friction coefficient, μ	0.3	(-)
Critical damping ratio, D (normal and shear)	0.3	(-)
Young's modulus, E_y	$2.5x10^6$	πρdg/6
Poisson's ratio, ϑ	0.3	(-)
Time step	0.00001	√(d/g)
Normal pressure	$1.4x10^6$	πρdg/6
Shear velocity	6.5	√(gd)

It can be clearly seen that for both spherical and ellipsoidal particles, there is a symmetric velocity field with small velocities at the central region, and the velocity gradually increases towards the moving platens with the maximum shear velocity at the regions near the platens. The variation of the velocity is due to the dissipative interaction forces between particles at the adjacent laminar layers. The movements of particles near the platens are mainly driven by the interaction forces between particles and the platens, causing large velocities. The particles in the central region move in the two flow directions, counterbalancing each other there, resulting in negligible velocities.

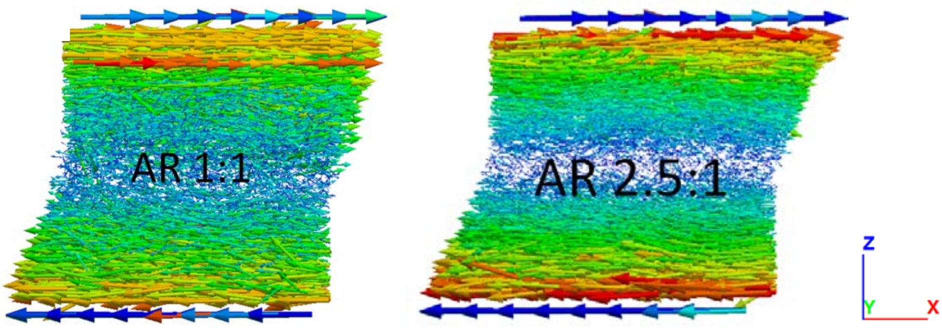

Fig. 4. Velocity fields for assemblies of particles (left: spherical; right: ellipsoidal with aspect ratio 2.5:1)

To have a clearer view, the time-averaged velocities of particles at different layers are analysed in Fig. 5a. Both ellipsoidal and spherical particle assemblies show similar linear velocity gradient with near-zero value at the central plane. The relative velocity is not 1 or -1, which indicates that there is a slip near the platens.

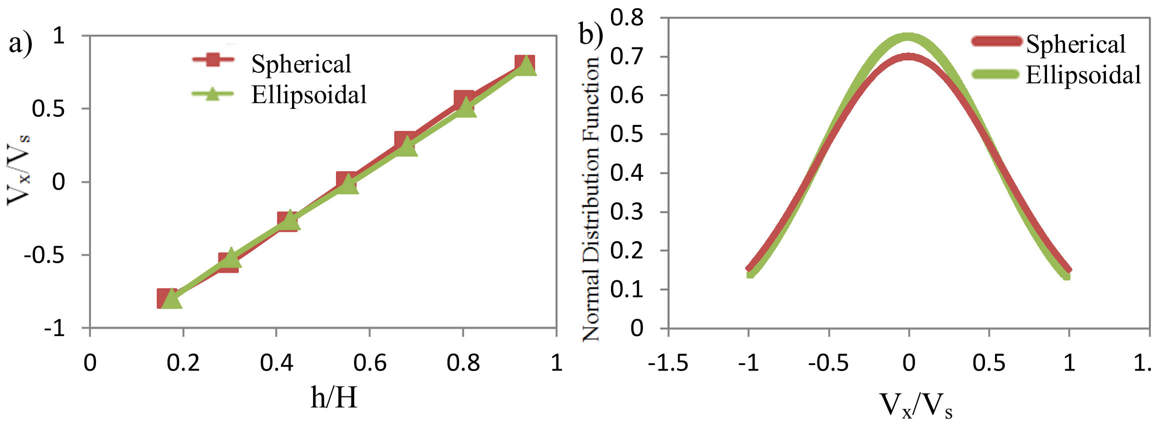

Fig. 5. a) Scaled velocity gradient along scaled height for spherical and ellipsoidal particle assemblies; b) normal distribution of scaled velocities with spherical and ellipsoidal particles. V_x and V_s are the average velocity of particles at a layer and shear velocity of the platens respectively, and h and H are the layer height and segment height respectively.

It is worth mentioning that the velocity gradient for shear cell is still an open question, even for spherical particles. While some studies [8] suggested there was a linear velocity profile, others found the velocity profile was non-linear [10]. It is a subject that needs further work but is beyond the scope of this paper.

Further, the statistical distribution of the particle velocity is shown in Fig. 5b for the two assemblies of particles. A clear symmetric Gaussian distribution of velocity can be seen with its peak at the zero velocity for both cases. In addition, the plot suggests that the velocity distribution of ellipsoidal particles has a higher peak at the mean value (zero) and lower dispersion away from the mean value, which implies that the number of stationary particles is higher for ellipsoidal particles. This phenomenon can be explained by particle alignment. As the particles become aligned with the direction of flow, the more elongated the particles are, the higher is the frictional surface between two laminar layers of the flow. This causes more energy dissipated and hence the peak increases at the mean velocity. In other words, the deviation of individual particle velocities from the mean value reduces with the elongation of particles.

3.3 COORDINATION NUMBER AND VOLUME FRACTION

In granular rheology analysis, coordination number and volume fraction are the two key parameters that are often utilized to understand the flow pattern. In this study, we consider the coordination number and volume fraction on the central plane of the segment perpendicular to the direction of flow. It was found that ellipsoidal particles have much higher coordination number and volume fraction than spherical particles.

The relationship between coordination number and volume fraction is of research interest in the precious studies [10]. The relationship is complex even for spherical particles, and related to particle properties, and operational and geometrical conditions. In general, it is non-linear in a large range. But for some cases, it is linear in a certain range. To study the feature for the systems considered here, more cases with higher normal pressures have been considered. As shown in Fig. 6, the two properties maintain positive relationship for spherical particles, as well as for ellipsoidal particles in the range of coordination number considered, i.e., between 0.59 and 6.3 for spherical particles, and 10.8 and 12 for ellipsoidal particles. Further comparison indicates that the variation gradient of the coordination number with volume fraction is higher for ellipsoidal particles.

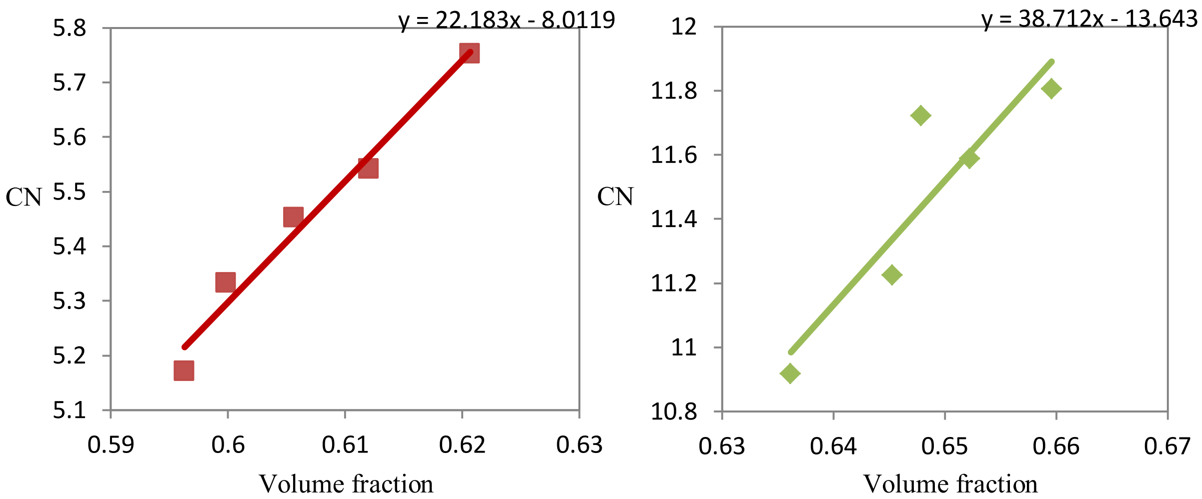

Fig. 6. Relationship between coordination number and particle volume fraction for spherical (left) and ellipsoidal (right) particles.

3.4 STRESS TENSOR ANALYSIS

In this section, stress tensors are microdynamically investigated for both cases of spherical and ellipsoidal particles. Fig. 7 shows the distributions of the stresses along the y axis direction. It can be seen that all stresses vary little along the y axis direction for the two cases. Of all the normal stresses, T_{zz} has the highest magnitudes, while T_{yy} the lowest. These results are similar to the findings in the previous studies of spherical particles [11]. The difference between the magnitudes of T_{yy} and T_{zz} for the two kinds of particles are not significant, due to the fact that the inter-particle forces in the y and z axis directions have similar values for the two cases. It can be clearly observed that T_{xx} for ellipsoidal particles is smaller than that of spherical particles while T_{xz} for ellipsoidal particles is higher than that of spherical particles. This is because the values of stresses are not only related to the values of the forces between particles, but also the directions of the branch vector connecting the mass centers of the particles in contact. Although the inter-particle forces in the x axis direction are larger for the case of ellipsoidal particles, the components of the branch vector in the x axis direction are much smaller, resulting in smaller stress T_{xx}. The components of the branch vector in the z axis direction are much larger, so the magnitude of the shear stress T_{xz} is higher for ellipsoidal particles.

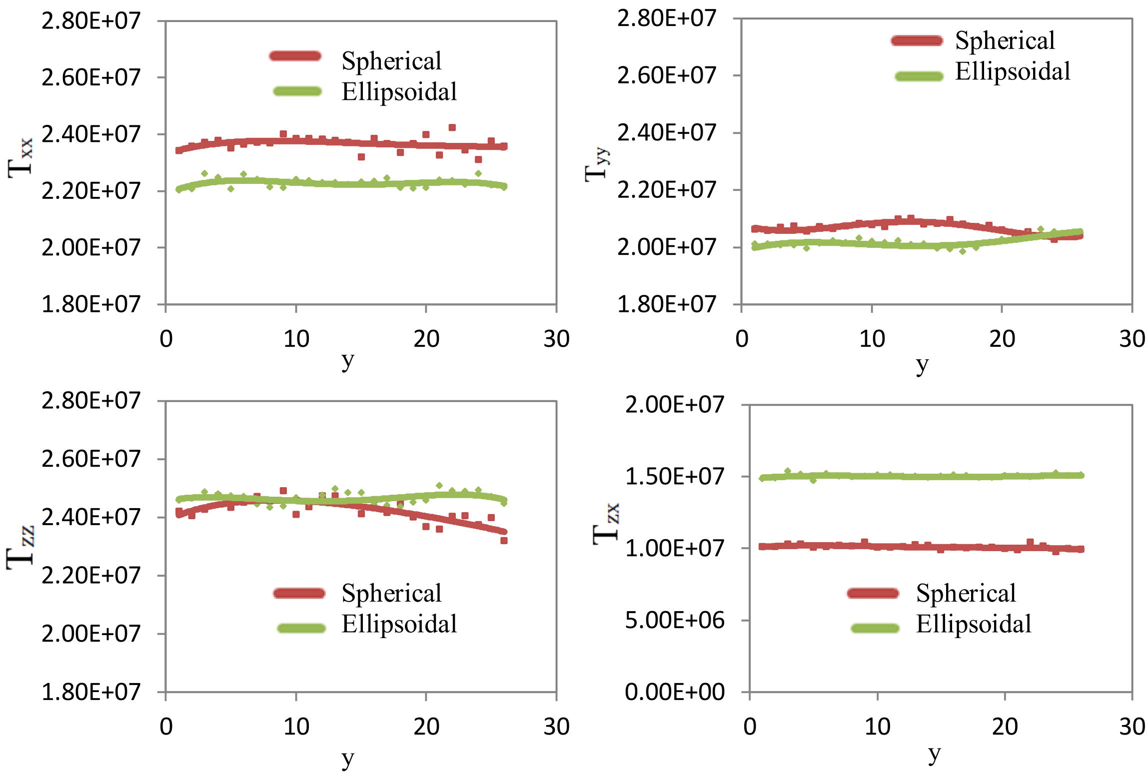

Fig. 7. Distributions of the stress tensor along the y- axis direction.

These stresses can be further analysed through their statistical distributions, as shown in Fig. 8. The trends are qualitatively similar to the result found for cohesive spherical particles in [11]. In all cases, it can be observed that ellipsoidal particle assembly has a higher peak but has less deviation from the mean. This is due to the particle alignment which orderly fashions the flow towards the direction of shear producing uniformity, and the force chains in ellipsoidal particle assembly which are created and destroyed less frequently than spherical particles. Normally, as the particles get more elongated, the weak force chains grow in percentage causing the less dispersion [12].

It is also observed that T_{yy} and T_{zz} for ellipsoidal particles have relatively higher peak while T_{xx} the lowest peak. This results from the fact that ellipsoidal particles are aligned with the flow direction (x-axis direction) and have less movements in the transverse directions (y- and z- axis directions), which causes more uniform distribution of T_{yy} and T_{zz}. On the other hand, the lowest peak of T_{xx} is attributed to the large impact of particles shearing in opposite directions, resulting in more deviation of T_{xx} from its mean value compared to other stresses.

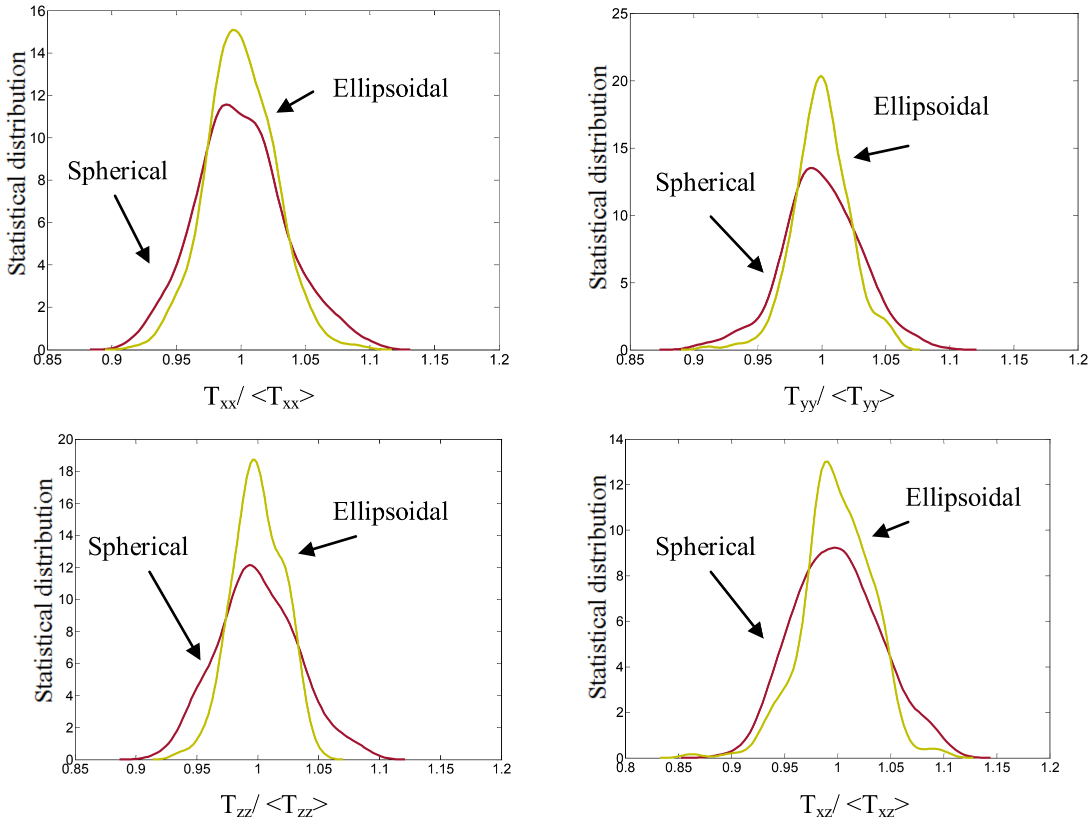

Fig. 8. Statistic distribution of the scaled stresses T_{xx}, T_{yy}, T_{zz} and T_{xz} in the yz-plane

4 CONCLUSION

While results on spherical particles assembly have been found to be qualitatively in agreement with the well-established knowledge, some interesting points have been identified demarking spherical and ellipsoidal particles. The major axes of ellipsoidal particles are approximately aligned with the direction of shear velocity of the flow, which is consistent with the previous studies. For both spherical and ellipsoidal particles, the linear velocity distributions are discovered. There is no significant difference for the two kinds of particles in terms of the velocity profile. Ellipsoidal particles have larger overall coordination number and volume fraction. Similar to spherical particles, the coordination number for ellipsoidal particles has a linear relationship with volume fraction. The stresses are also influenced by the shape of ellipsoidal particles. Especially, the ellipsoidal particle assembly has a much higher shear stress than spherical particles. Overall, ellipsoidal particle assembly has less dispersion in the distributions of velocity and stresses compared with spherical particles.

5 REFERENCES

[1] Carr, J. and Walker D. An annular shear cell for granular materials. *Powder Technology* (1968) **1**(6): 369-373.

[2] Cundall, P. A. and Strack, O. D. A discrete numerical model for granular assemblies. *Geotechnique* (1979) 29(1): 47-65.

[3] Zhu, H.P., Zhou, Z.Y., Yang, R.Y. and Yu, A.B. Discrete particle simulation of particulate systems: A review of major applications and findings. *Chemical Engineering Science* (2008) **63**: 5728 - 5770

[4] Hertz, H. Uber die Beruhrung fester elastischer Korper. *Journal für die reine und angewandte Mathematik* (1881) **92**: 156-171.

[5] Deresiewicz, H. *Effects of an oscillating torsional couple on the contact surfaces of elastic spheres.* No. CU-TR-5. Columbia University of New York Dept. of Civil Engineering and Engineering Mechanics, (1953).

[6] Zhu, H.P., Zhou, Z.Y., Yang, R.Y. and Yu, A.B. Discrete particle simulation of particulate systems: Theoretical developments. *Chemical Engineering Science* (2007) **62**: 3378 – 3396

[7] Guo, Y., Wassgren, C., Hancock, B., Ketterhagen, W. and Curtis, J. Granular shear flows of flat disks and elongated rods without and with friction. *Physics of Fluids* (2013) **25**(6): 063304.

[8] Campbell, C. S. Stress-controlled elastic granular shear flows. *Journal of Fluid Mechanics* (2005) **539**(-1): 273.

[9] Taghavi R. Automatic clump generation based on mid-surface. In: D. Sainsbury et al. (eds). *Continuum and Distinct Element Modelling in Geomechanics*. Itasca, Minneapolis (2011) pp. 791-797.

[10] Wang, X. Zhu, H. P. and Yu, A. B. Microdynamic analysis of solid flow in a shear cell. **Granular Matter** (2012) 14(3): 411-421.

[11] Aarons, L. and Sundaresan S. Shear flow of assemblies of cohesive granular materials under constant applied normal stress. *Powder Technology* (2008) **183**(3): 340-355.

[12] Az´ema E. and Radja¨i, F. Stress-strain behaviour and geometrical properties of packings of elongated particles. *Physical Review E* (2010) **81**: 051304.