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Particle Alignment and Volume Fraction for Ellipsoidal Particles

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Abstract

This paper studies rheological properties of elongated ellipsoidal particles in a model annular shear cell in stress controlled flow condition using the discrete element method (DEM). Particle orientation and volume fraction of the flow are considered. Probability distribution of particle orientation angle exhibits the effect of different shear rates as such that at lower shear rates there is a systematic increase in number particles aligned to the direction of flow with the increase of load, which is not found in the study of higher shear rates. Then, a correlation between orientation angle and volume fraction for different shear rates is observed. It shows that, for the particle assembly volume fraction above 0.55, there is a noticeable influence of shear rate on the relationship between orientation angle and volume fraction. For volume fraction below 0.55, the relationship curve collapse into a single curve indicating that the relationship is no longer affected by variation of shear rate. This observation has a similar pattern with the correlation between kinetically scaled stress and volume fraction, which has been used to determine the transition between kinetic and intermediate regime for spherical particles.

Keywords: Granular materials, rheology, discrete element method, shear cell, ellipsoidal particle

1. INTRODUCTION

Granular rheology is an important topic of research because of its extent of existence in human society. Food products like grain and salt, finished metal products like nuts and bolts, mineral products like coals and limestones, all fall under the category of granular materials. So, the study of handling of such materials is essential from industrial perspective as better control of this activity will lead to significant economic and operational benefits. However, it is a complex phenomenon and is quite difficult as well as expensive to study through experimental method. Consequently, alternative numerical methods such as the discrete element method (DEM) have been developed, which allows the study of this phenomenon in virtual environment with much ease.

The DEM is based on the simple Newton's law of motion which tracks interactions among particles with respect to force and velocity. Because of its comprehensiveness, the demand for computational resources is very high. For this reason, earlier numerical studies on granular rheology were predominantly on spherical particles (Campbell and Brennen (1985)). While acknowledging the fact that these investigations provide enormous contribution to this field, they are distant from practical scenario which consists of non-spherical particles. With the development of computational technology in the modern era, it is now possible to address the issues with respect to non-spherical particles as well, which has motivated current researchers to incline more towards study of non-spherical particles (Campbell (2011)).

Particle alignment is a special feature of elongated non-spherical particles in the field of granular rheology. It is unique to non-spherical particles as it has no meaning for spherical particles because of their isotropic shape. Our previous study of ellipsoidal particles showed that particle preferential alignment plays an important role governing the flow mechanism of the assembly (Hossain et al. (2015)). Similar result has also been found in other numerical work (Guo et al. (2013)) and experimental studies (Börzsönyi et al. (2012)) for other elongated non-spherical particles such as rods and disks. Volume fraction of granular assembly is of special interest in the previous studies (e.g. Abeles et al. (1975), Hanes and Inman (1985)), it is an important property to identify regime transition points in granular rheology (Campbell (2005), Aarons and Sundaresan (2008), Wang et al. (2013)). However, the relationship of particle alignment and volume fraction has not been investigated in the past.

In this paper, novel research has been performed in a numerical platform using the discrete element method (DEM) on ellipsoidal particle assembly that are placed inside an annular shear cell in a pressure controlled environment. The assembly is subjected to different mix of externally applied pressure and induced shear. The probability distributions of particle orientation angle for different applied loads and shear velocities are examined. Then, the relationship between particle orientation angle and assembly volume fraction is studied.

2. SIMULATION METHOD AND CONDITIONS

In this work, granular rheological analysis is performed by means of the DEM using spring dashpot model for soft particle simulation. The software package PFC3D 5.0 is utilized to simulate the flow of ellipsoidal particles in a 3D annular shear cell. The non-linear model based on Hertz-Mindlin and Deresiewicz model is used to calculate the contact forces between particles. The details on the DEM can be seen elsewhere (refer to PFC Help File).

A rectangular segment of widely studied annular shear cell is considered for the ellipsoidal particles (Figure 1a) here. The segment has a dimension of 11d ×11d × H, where d is the effective diameter of ellipsoidal particles (effective diameter is the diameter of a spherical particle with same volume of ellipsoidal particle being studied) and H is the height of the upper platen. The segment has two periodic boundary planes perpendicular to the x-axis. 121 spherical particles of 1.0d diameter are used to constitute each of the upper and lower platens of the segment so that the entire area of the platens is filled. The particles forming the platens possess the same physical properties (such as density, damping coefficient, friction coefficient and stiffness) as other particles.

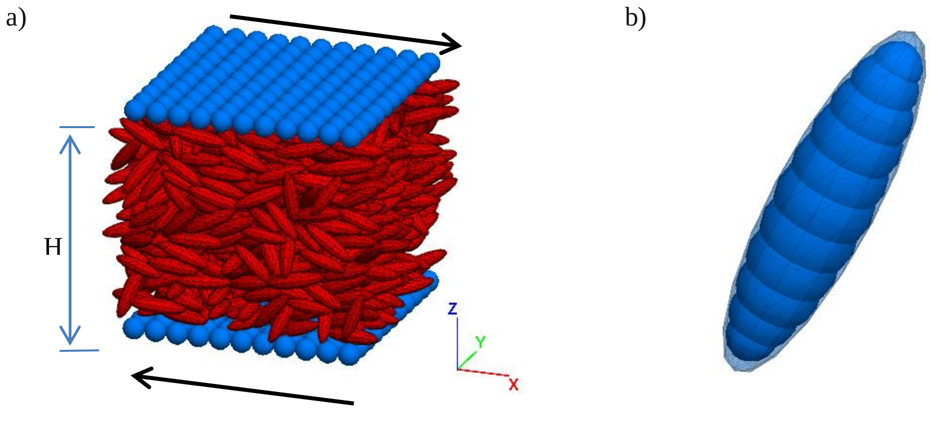


Figure 1. a) Simulated model shear cell; b) construction of ellipsoidal particle

The ellipsoidal particles considered have an aspect ratio of 3.75:1. Bubble-pack algorithm (Taghavi (2011)) is used to construct these particles (Figure 1b) in this work. The closed surface of the non-spherical particle is first constructed with triangular meshes of various sizes. Spherical particles of various sizes are then used to fill the space within the surface to obtain a specific volume. These particles are then glued and made immobile relative to each other and thus the particle of desired shape is constructed.

In each simulation, 1000 slightly poly-disperse particles are first generated randomly between the upper and lower platens with an initial volume fraction of 0.7. Their effective diameter ranges from 0.9~1.1d. 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 gradually increased by moving upper and lower platens in opposite direction to the pre-set value after the loading has been stabilized. When the system becomes steady, the process of collecting relevant data starts. The particle properties and simulation parameters are given in Table 1.

It is worth mentioning that gravity was not considered here, similar to some of the previous studies (e.g., Aarons and Sundaresan (2008)). Normally, gravity affects the dynamic behaviors of shear flows. However, when the pressure applied by upper platen is high enough for the system considered in this work, as suggested by our previous work (Hossain et al. (2016)), the effect of gravity would not impact the granular flow.

TABLE 1: Particle properties and parameters used in the simulations

Property	**Value**	**Unit**
Particle friction coefficient, μ	0.3	(-)
Critical damping ratio, D (normal and shear)	0.1	(-)
Young's modulus, Ey	2.5×10^6	$\pi\rho dg/6$
Poisson's ratio, ϑ	0.3	(-)
Time step	0.00001	$\sqrt{(d/g)}$
Normal pressure, P	1.64-16352	$\pi\rho dg/6$
Shear velocity, γ	1.07-12.8	$\sqrt{(gd)}$

3. RESULTS AND DISCUSSION

Figure 2 shows the particle preferential alignment in the direction of the flow. It can be observed that the ellipsoidal particles have their major axis aligned in the direction of shear (here, direction along the x-axis). Similar observation was obtained in the studies of Reddy et al. (2009), Börzsönyi et al. (2012), and Guo et al. (2013).

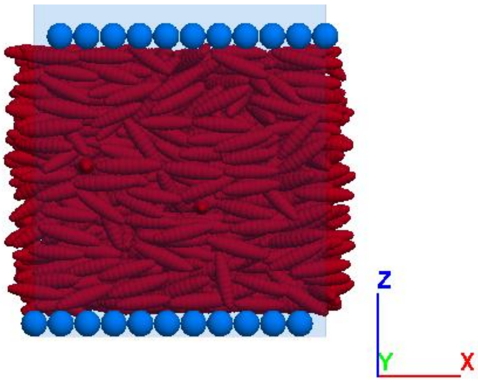


Figure 2. Illustration of particle preferential alignment in the direction of flow

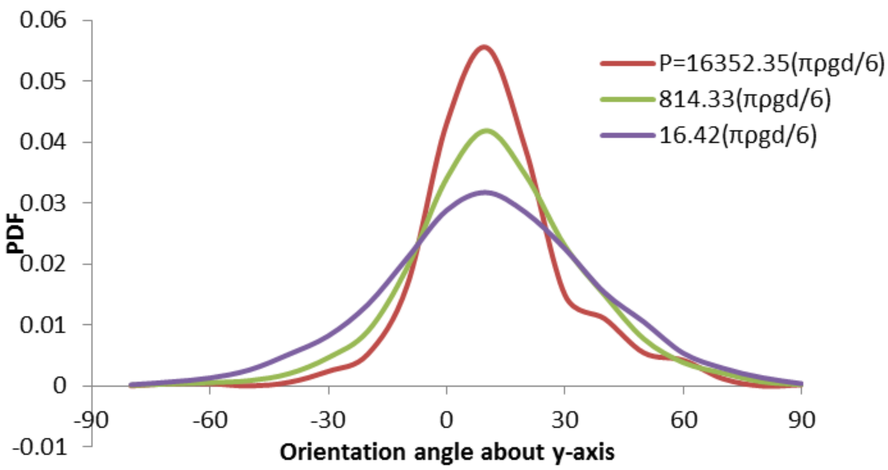
Figure 3 shows the probability distribution of particle orientation angle (between -90 and +90 degree about the y-axis) for different applied loads and different shear velocities. The distribution curves for different shear velocities are presented separately to avoid clutter. Regardless of load and shear combination, all curves are found to be of Gaussian nature with their peak slightly higher than zero degree angle. In application, it means that more particles are aligned in the direction of flow which causes the angle of the particles about the y-axis to be near zero. It is in agreement with results of the experiment by Börzsönyi et al. (2012), as well as numerical analyses by Guo et al. (2013).

However, the interesting thing to note here is that at low shear velocity ($1.07\sqrt{gd}$), as shown in Figure 3a, there is a very clear effect of variation of shear rate on the particle alignment statistics. When particle assembly is subjected to high applied load, more particles are aligned towards the flow. As the applied load is reduced for the same shear velocity, the tendency of preferential alignment for the particles in flow direction reduces. The reduction follows a systematic gradual trend. On the other hand, variation of load on particle assembly subjected to higher shear has less noticeable effect on particle preferential alignment.

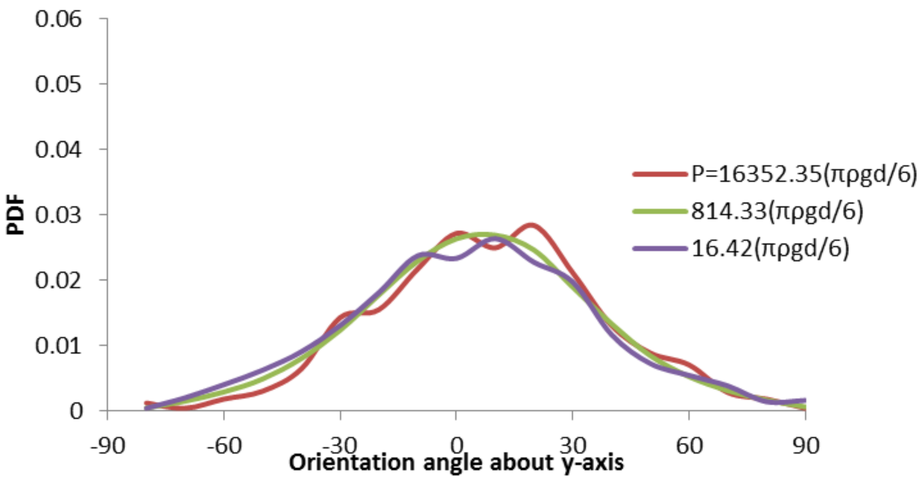
The physical reason can be understood from the existing work of spherical particles (Wang et al. (2012)). Shear velocity for ellipsoidal particles has strong influence on volume fraction of the assembly. Volume fraction is lower for higher shear velocity. It is because when the particles of the assembly are at higher shear rate, shear force is also higher. This shear force contributes to the force exerted by adjacent particles to the upper platen. In response, the upper platen rises higher to maintain constant stress on the particle assembly. As a result, overall volume fraction reduces and particles are more relaxed to obtain alignment away from flow direction for higher shear velocity. On the other hand, at a low shear, volume fraction increases with increase of applied load in a systematic manner because the contributory resistant force on upper platen derived from low shear force is less effective. Hence, particles at low load are more able to disperse further from preferential alignment due to low volume fraction. And this ability systematically reduces when the load is increased and consequently volume fraction increased making particles less able to disperse away from preferential alignment position during flow.

Further, Figure 4 shows the relationship between the time-averaged particle orientation angle about the y-axis and the time-averaged overall assembly volume fraction at different induced shearing velocities. We find a data collapse in the correlation curves below the assembly volume fraction of 0.55 similar to the volume fraction at which granular rheology transits between inertial and intermediate regime. It means that, below 0.55 volume fraction, variation of shear rate does not affect the relationship between particle alignment and volume fraction. But above 0.55 volume fraction, the effect of shear velocity variation becomes apparent as particle orientation angle reduces at higher volume fraction in contrast to the orientation angle at higher shear velocity. We find that there is a similarity between this relationship and the relationship between kinetically scaled load and volume fraction (Hossain et al. (2017), Aarons and Sundaresan (2008), Wang et al. (2013)) that is used to identify regime transition of granular rheology. This is a new approach in light of regime transition and motivates further research in this aspect in the future.

a)



b)



c)

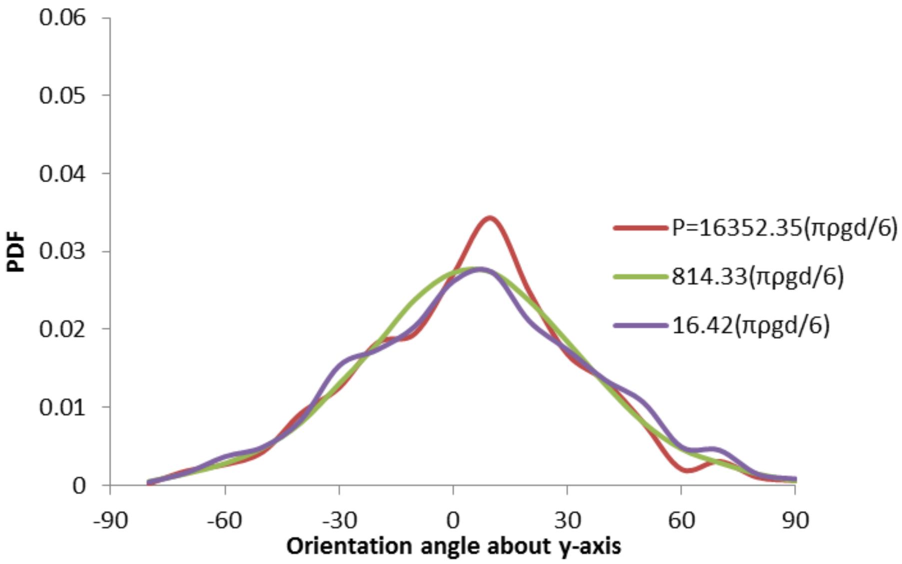


Figure 3. Probability distributions of particle orientation angle about the y-axis for particle assembly subjected to different loads at shear rates: a) $1.07\sqrt{gd}$, b) $4.02\sqrt{gd}$, and c) $12.8\sqrt{gd}$.

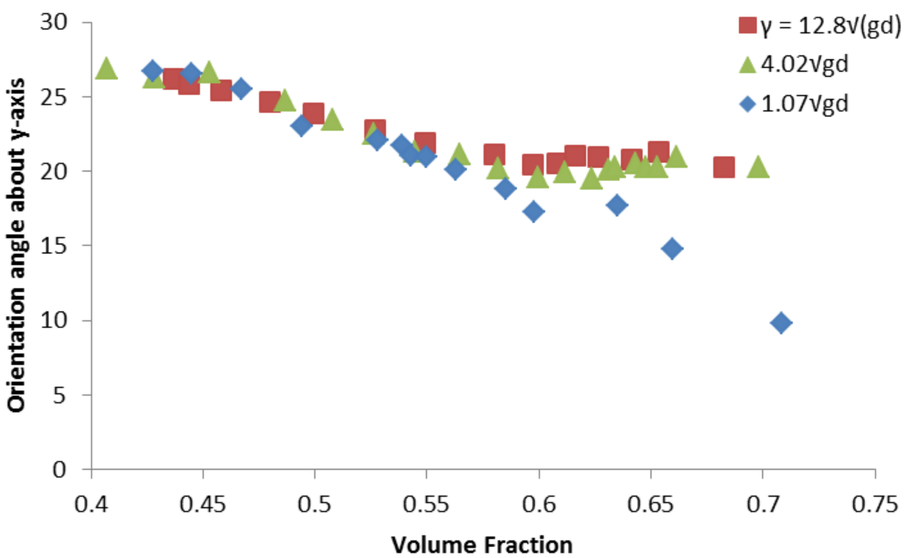


Figure 4. Relationship between particle orientation angle and volume fraction for different induced shear velocities.

4. CONCLUSION

Granular rheology of ellipsoidal particle assembly is investigated in a stress controlled flow through annular shear cell in a simulated environment based on numerical approach of DEM. A study of probability distribution shows there is a systematic graduation of increase of peak for orientation angle at a near zero value with the increase of externally applied load which is not so profound at higher shear velocity. A physical interpretation is drawn from the understanding of relationship between volume fraction and preferential alignment: at low shear rate, the overall volume fraction is low at low load providing more room for constituent particles to be further from preferential alignment position. This room reduces as volume fraction increases with the increase of load and the particles are more aligned. This is not the case with particles with higher shear rate where contribution of shear rate balances the impact of upper platen to some extent. Relationship between particle orientation angle and volume fraction is obtained for different induced shear velocities. An interesting new finding achieved that shows a collapse of data for the correlation curves below a volume fraction similar to that of regime transition for inertial regime suggesting there is no effect of variation of shear rate on particle preferential alignment below this volume fraction.

5. ACKNOWLEDGMENTS

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