

# IMPORTANCE OF PERIODIC BOUNDARIES OR FRICTIONLESS WALLS IN SIMULATING ELEMENTARY RESPONSE OF ANGULAR PARTICLES

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**Abstract.** *In the discrete element method (DEM), the granular response is affected by the selection of boundary conditions, thereby emphasizing the importance of their careful consideration [1]. Replicating the boundary conditions employed in experiments is crucial to have a quantitative agreement between the response observed in the simulation and laboratory test [2]. In this study, a calibrated and validated DEM model was utilized to perform a series of simulations featuring regular polygons with varying numbers of corners subjected to different boundary conditions. The aim was to examine the combined effect of particle shape and boundary conditions on the mechanical response of granular assemblies. Simulations were performed under three boundary conditions: rigid frictional walls (in which the friction between the particle-wall interface is equal to that between the particle-particle interface), rigid frictionless walls, and periodic boundary conditions (PBC). Interestingly, it was observed that qualitatively, the effect of particle shape on granular response was invariant, irrespective of boundary conditions employed. However, quantitatively, the shear strength of all shapes was significantly affected by boundary settings, with the maximum and minimum strengths exhibited under rigid frictional walls and periodic boundaries, respectively. The magnitude of the decrease in shear strength due to boundary conditions was contingent upon the particle shape, with angular assemblies demonstrating a significant change in strength relative to round assemblies. Angular particles in contact with rigid wall frictional boundaries exhibited lesser rotations, thereby inducing relatively significant shear forces on the walls, particularly those parallel to the shearing direction. On the other hand, round particles in contact with walls rotated to a greater extent, resulting in little or negligible shear forces with the walls. Furthermore, boundary conditions also affected deformation patterns, including the development of shear bands.*

## 1 INTRODUCTION

The large-scale behavior of granular materials is influenced by small-scale mechanisms that occur at the particle level, owing to their discrete nature [3]. Particle characteristics such as size, size distribution, and shape primarily govern these particle-scale mechanisms [4,5]. Among these characteristics, the particle shape has garnered significant attention from researchers in recent decades [6–8]. This focus has helped us understand that particle shape is a key factor in controlling the spatial arrangement of particles and exerts a significant influence on the mechanical response of granular materials [9]. However, traditional laboratory investigations face challenges in effectively controlling particle shape and measuring particle-level mechanisms. As an alternative approach, the discrete element method (DEM), introduced by Cundall [10], has emerged as a powerful tool for investigating the mechanical behavior of granular materials [11,12]. It allows for the explicit modelling of discrete particles with diverse shapes, facilitating the direct observation and analysis of particle-level mechanisms [13]. This method often proves more convenient compared to conventional laboratory investigations. Consequently, many researchers have directed their attention towards exploring the effects of particle shape especially on particle-level mechanisms using DEM, contributing valuable insights to enhance our understanding of granular behavior [14].

In DEM, the choice of boundary conditions significantly affects the granular response. Two popular boundary conditions are rigid walls and periodic boundary conditions (PBC). Among these, PBC have been recognized as the most effective treatment for eliminating wall effects while maintaining a continuous internal flow involving particle-particle contacts throughout the computational domain [1]. Replicating the boundary conditions employed in experiments is crucial for achieving quantitative agreement between simulation results and laboratory tests [2]. For instance, in geotechnical engineering, the widely used conventional triaxial test utilizes flexible membranes as lateral boundaries, allowing for non-uniform lateral displacements and the formation of clear shear bands. To replicate similar boundary conditions in DEM simulations, researchers have employed hydrostatic boundaries [12,15], mixed boundary conditions [2], and collections of small balls [8] to enable non-uniform lateral deformations.

To date, the interactions between particle shape and the chosen boundary conditions have not been thoroughly investigated. Therefore, the specific manner in which particle shape and boundary conditions collectively impact the behavior of granular materials within the DEM framework remains unexplored. This knowledge gap highlights the need for further investigation to comprehensively understand how these two factors interact and contribute to the overall mechanical response of granular materials in DEM simulations.

In this study, we conducted DEM simulations using polygon-shaped particles with different numbers of corners (representing different particle roundness) under different boundary conditions. The primary objective of this study was to address two research questions: 1) Does the influence of particle roundness on the mechanical response of a granular system remain consistent regardless of the chosen boundary conditions? and 2) Does the impact of boundary conditions on the mechanical response of a granular system remain consistent regardless of particle roundness? By exploring these questions, we aimed to gain insights into the relationship between particle roundness, boundary conditions, and the resulting mechanical behavior of granular materials.

## 2 DEM SIMULATION SETUP

In this study, we utilized the two-dimensional discrete element method (DEM) model of the biaxial shearing test, which was originally developed by Ali et al. [16] using PFC2D. The DEM model involved a square box with initial dimensions of 350mm x 350mm. The Hertz contact model was employed to represent the interactions between particle-particle and particle-boundary contacts. The material parameters used in the simulation are shown in Table 1 remaining consistent with those reported in [16].

### 2.1 Granular sample generation

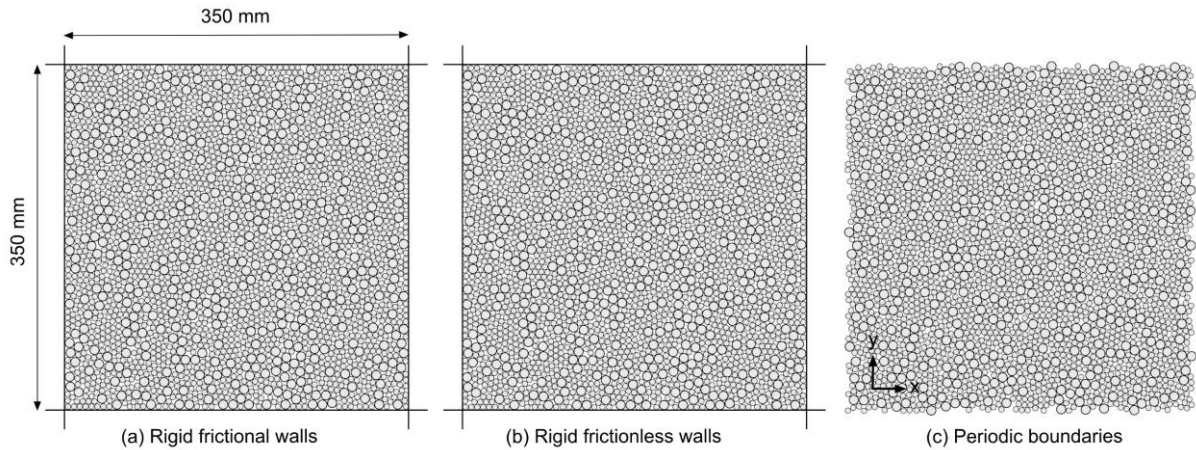
The simulations employed granular samples comprising non-elongated convex-shaped polygonal particles. These particles were created into single-shaped dual-size samples through a radius expansion method. Two sizes of polygonal particles were generated: those with inscribed diameters of 10mm and 6mm. The ratio of larger to smaller particles was maintained at 2:3 by volume across all samples. The required number of particles were placed in the biaxial box with their sizes smaller than the actual sizes, subsequently, the particles underwent expansion. During this expansion, interparticle friction was set to zero, and the sample was cycled until an equilibrated state with the desired porosity was achieved. All samples were generated with the same initial void ratio i.e., 0.2. The samples comprise approximately 2400 to 2700 particles.

### 2.2 Boundary conditions

Three distinct boundary configurations, as depicted in Figure 1, including rigid frictional walls, rigid frictionless walls, and periodic boundaries were employed. Ali et al. [16] utilized rigid frictional walls in their original DEM model to replicate their experimental boundary conditions for precise calibration and validation purposes. For this, friction between particle-wall was considered to be the same as particle-particle. They briefly touched upon results with periodic boundaries as well. However, their primary focus was investigating the systematic impact of particle roundness. This study places greater emphasis on understanding the interplay between different particle shapes and various boundary conditions, and how this interaction influences the overall response of granular materials. Therefore, in addition to rigid frictional walls and periodic boundaries, we also considered the inclusion of rigid frictionless walls in our investigation. By incorporating all three boundary settings, we aim to provide a comprehensive analysis of how different particle shapes and boundary conditions contribute to the observed granular behavior.

**Table 1.** DEM model contact parameters with different boundary conditions.

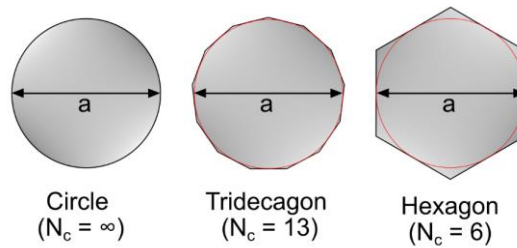
Parameter	Frictional walls	Frictionless walls	Periodic space	Unit
Particle density, $\rho$	2710	2710	2710	Kg/m <sup>3</sup>
Particle-particle friction, $\mu_{p-p}$	0.2	0.2	0.2	
Particle-wall friction, $\mu_{p-w}$	0.2	0.0	-	
Shear modulus, $G$	26.0	26.0	26.0	GPa
Poisson's ratio, $\nu$	0.3	0.3	0.3	
Local damping parameter	0.2	0.2	0.2	



**Figure 1.** DEM models with different boundary conditions (a) Rigid frictional walls (b) Rigid frictionless walls (c) Periodic space

### 2.3 Particle shapes

The shearing response of three polygonal shapes of different numbers of corners ( $N_c$ ) including circle, tridecagon, and hexagon was simulated. The circle with  $\infty$  corners represents highly rounded particles, the tridecagon with 13 corners represents moderately round particles, and the hexagon with 6 corners represents highly angular particles. The particle shapes are selected to cover a wide range of particle roundness. To link particle shape and mechanical parameters of granular materials, it is essential to quantify the particle shapes using an appropriate shape index. For this, the roundness ( $R$ ) of each polygon was determined using Wadell's roundness definition.  $R$  is defined as the ratio of the average radius of curvature of the corners to the radius of the maximum inscribed circle [17].  $R$  is computed for each polygon using 2D binary images (600 dpi image resolution) and algorithms based on Wadell's definition [18]. The value of  $R$  for circle, tridecagon, and hexagon was 1.0, 0.50, and 0.15, respectively. Figure 2 shows the shape of the particles used.



**Figure 2.** Particle shapes used in this study

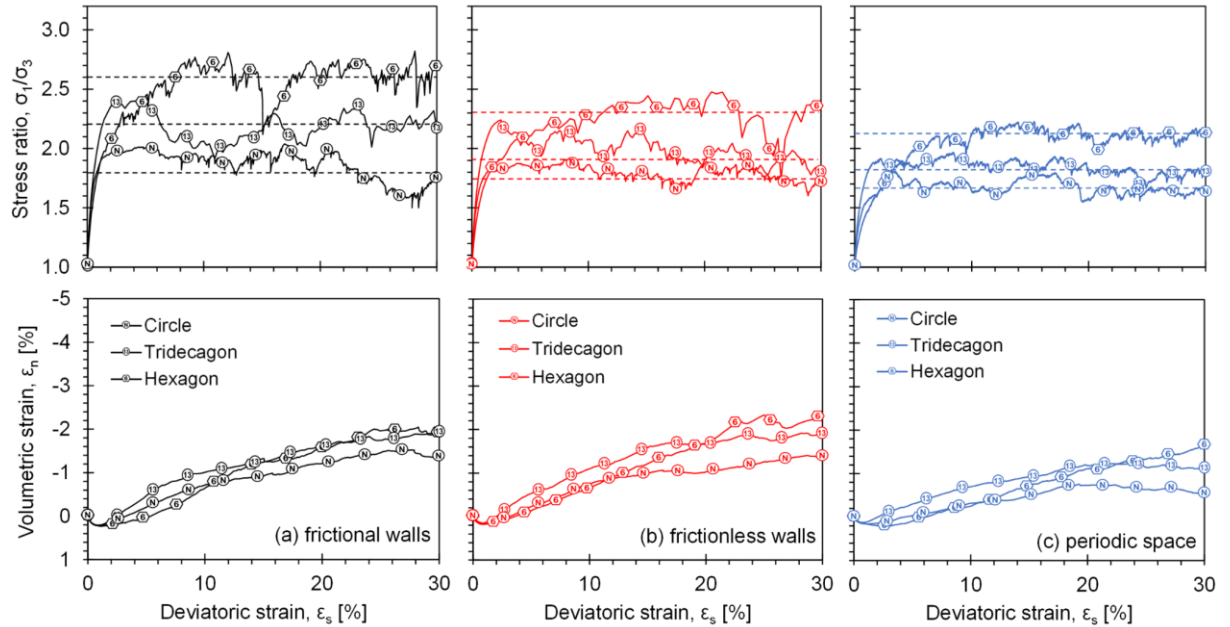
### 2.4 Simulation procedure

The simulations are divided into two main phases: an initial isotropic compression phase followed by a shearing phase. In the isotropic compression phase, the sample is compressed under  $\sigma_1 = \sigma_3$  condition, until the desired confining pressure is achieved. Once the isotropic compression is completed, the shearing phase commences. During the shearing phase, a servo

control system is employed to maintain a constant confining pressure. The top wall is then incrementally moved downward in a normal direction at a constant axial strain rate. The inertial number ( $I$ ) was maintained lower than  $7.8e-5$  in all simulations which ensures quasi-static shearing. The shearing phase is performed at three different confining pressures ( $\sigma_3 = 19.6, 39.2,$  and  $58.8\text{kPa}$ ). In the following, the mean normal stress and the deviatoric stress are expressed as  $p = (\sigma_1 + \sigma_3)/2$  and  $q = \sigma_1 - \sigma_3$ , where  $\sigma_1$  and  $\sigma_3$  are principal stresses in the  $y$  and  $x$  directions, respectively. Volumetric strain and deviatoric strain are defined as  $\varepsilon_n = \varepsilon_1 + \varepsilon_3$  and  $\varepsilon_s = \varepsilon_1 - \varepsilon_3$ , where  $\varepsilon_1$  and  $\varepsilon_3$  are principal strains in the  $y$  and  $x$  directions, respectively.

## 2.5 Calibration and validation of DEM model

Ali et al. [19] conducted biaxial experiments using schneebeli rod material with cross-sectional circular and hexagonal shapes. In addition to studying macroscopic stress-strain relationships, they employed a novel 2D image analysis technique developed by [20] to observe particle kinematics such as particle rotations and coordination numbers. Subsequently, Ali et al. [16] utilized these experimental findings to calibrate and validate the corresponding 1:1 scale DEM model. To achieve calibration, the behavior of circular particles was simulated and compared with the macroscopic stress-strain response and microscopic particle rotations of circular particles observed in the biaxial experiments. Next, the model was validated by simulating the behavior of hexagonal particles and comparing it with the experimental dataset of hexagonal particles. Through this calibration and validation process, they confirmed that the DEM model successfully captured the influence of particle shape on both macroscopic and microscopic particle-level mechanisms. For more detailed information about the calibration and validation of the DEM model, see Ali et al. [16].

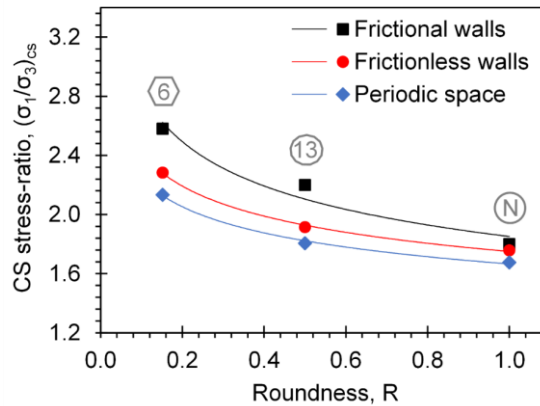


**Figure 3.** Effect of particle shape on stress-strain characteristics under various boundary conditions (a) frictional walls (b) frictionless walls (c) periodic space (dotted lines represent average stress ratio between 10% - 30%  $\varepsilon_s$ )

### 3 RESULTS AND DISCUSSION

#### 3.1 Stress-strain characteristics

Figure 3 illustrates the stress-strain relationships of three particle shapes under different boundary conditions. These simulations were conducted at a confining pressure ( $\sigma_3$ ) of 39.2 kPa. In general, the behavior of a granular system is observed to have maximum shear strength and volumetric dilations when frictional rigid walls are employed as boundaries. Conversely, the minimum strength and dilations are observed in cases where periodic boundaries are used. The extent of change in the strength of a granular system, resulting from variations in boundary conditions, is found to be dependent on the shape of the particles within the system. Figure 4 shows the comparison of critical state stress ratio  $(\sigma_1/\sigma_3)_{cs}$  (average from 10% to 30%  $\epsilon_s$ ) of all shapes under different boundary conditions. For example, when circular particles are considered, the change in  $(\sigma_1/\sigma_3)_{cs}$  is relatively minor. However, as the angularity of the particles increases, such as in the case of tridecagon particles, the change becomes more significant. The most angular particle shape used, the hexagon, exhibits the greatest change in  $(\sigma_1/\sigma_3)_{cs}$ . This emphasizes that while the effect of boundary conditions is qualitatively similar across different granular systems, the quantitative impact depends on the shape of the particles within the system. Angular particles are more susceptible to the influence of changing boundary conditions, experiencing a relatively higher level of impact. To discuss this shape-dependent variation, particle scale data is observed and analyzed in the following sections.



**Figure 4.** Relationship between critical state stress ratio and particle roundness for different boundary conditions

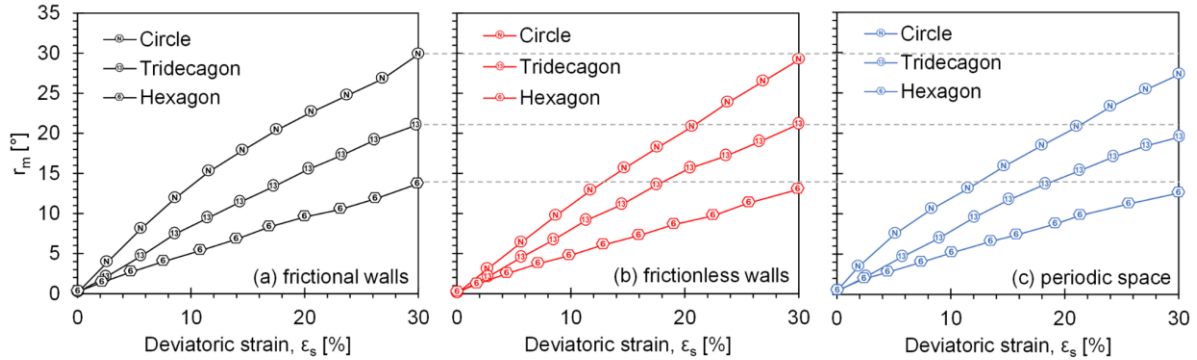
#### 3.2 Overall particle rotations

Particle rotations are recognized as pivotal mechanisms in granular deformations, primarily controlled by particle shapes and exerting a substantial impact on the mechanical behavior of granular materials. Consequently, it becomes crucial to explore the influence of diverse boundary conditions on the rotational behavior of particles with various shapes. For this, we quantify the absolute average cumulative rotations ( $r_m$ ) of all particles, defined as follows:

$$r_m = \frac{\sum_{i=1}^N |\theta_i|}{N} \quad (1)$$

where  $\theta_i$  is the cumulative rotation of an individual particle and  $N$  is the total number of

particles in the sample. Figure 5 shows the relationship between mean absolute cumulative rotation ( $r_m$ ) and deviatoric strain ( $\epsilon_s$ ). It is observed that particle shape has a significant influence on the rotational response of particles in such a way that round particles exhibit significantly higher while angular particles are relatively resistant to rotations. Similar effects of particle shape on rotational response have been reported by many researchers [14,16,19,21, 22].

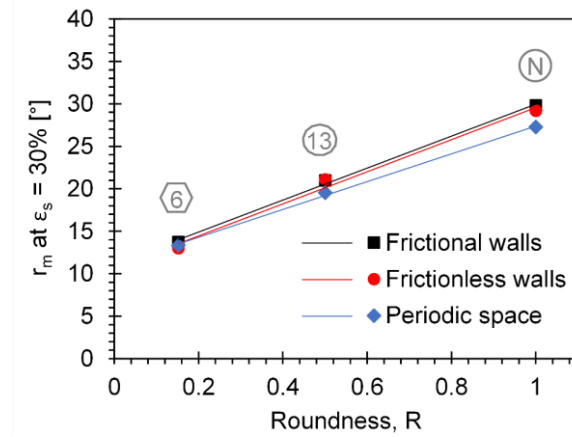


**Figure 5.** Mean absolute cumulative rotation ( $r_m$ ) evolution with deviatoric strain ( $\epsilon_s$ ) ( $\sigma_3 = 39.2$  kPa) (a) frictional walls (b) frictionless walls (c) periodic boundary

Even though the magnitude of particle rotations depends on the amount of shearing, the comparison of particle rotation magnitude at the same strain level provides a good overview to discuss the effect of particle shape and boundary condition. Therefore, the  $r_m$  value of all shapes at around 30%  $\epsilon_s$  is compared in Figure 6. Regardless of the boundary conditions, the qualitative effect of particle shape on rotational behavior is similar i.e., rotations increase with roundness. For a given shape, it can be seen that particle rotations are higher with rigid frictional boundaries and lowest with periodic boundaries. High particle rotations under rigid frictional boundaries occur because higher dilations cause a decrease in mean coordination number allowing particles to rotate easily. However, this effect caused by boundary conditions on rotational response varies based on the shape of the particles. For example, the difference between the  $r_m$  value for rigid frictional and periodic boundary is relatively significant for circular particles and decreases as the particles become more angular.

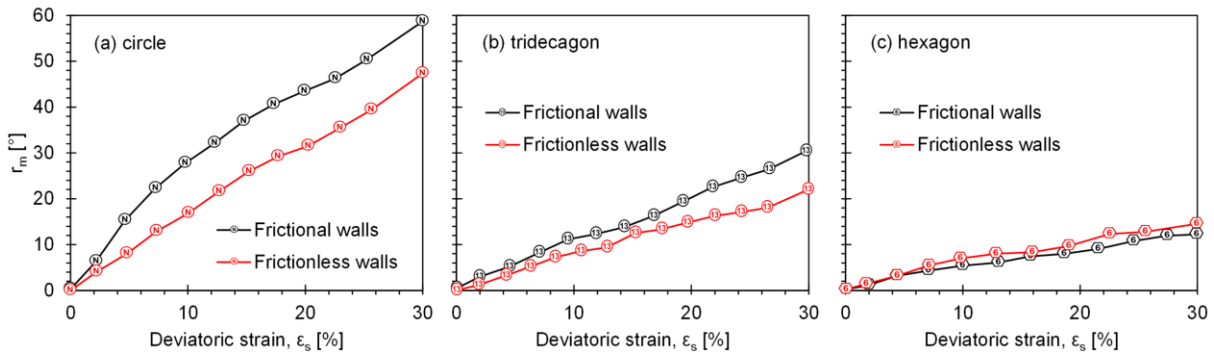
### 3.3 Rotations of particles in contact with rigid walls

Figure 7 shows the  $r_m$  and  $\epsilon_s$  relationship for particles that are in contact with boundaries. Particles that are in contact with rigid walls are referred to as rigid-wall-contacting (RWC) particles. These RWC particles are identified when the  $\epsilon_s$  was 30%, and their rotation history is subsequently traced backward during the shearing process. In general, the rotational behavior of RWC particles is found to be influenced by the shape of the particles in such a way that when round particles come into contact with the boundary, they tend to display significantly higher rotations. On the other hand, as the particles become more angular, the rotations decrease. To investigate the impact of surface friction of rigid walls, the relationship between  $r_m$  and  $\epsilon_s$  is plotted for each particle shape under two scenarios: simulations with and without surface friction applied to the rigid walls.



**Figure 6.** Comparison of  $r_m$  value of different shape shapes under various boundary conditions at  $\epsilon_s = 30\%$

Figure 7a illustrates that the rotations of RWC circular particles exhibit a significant increase when surface friction is introduced to the walls. This behavior can be attributed to the absence of rolling resistance in circular particles. Consequently, when shear forces occur between a circular particle and the wall, it initiates particle rotation, thereby preventing the generation of substantial shear forces. As a result, the effect of frictional boundaries on the shear strength of circular particles is found to be not significant. The qualitative effect of boundary friction on tridecagon particles exhibits similarities to that of circular particles. However, due to the relatively higher angularity of tridecagonal particles, the magnitude of the boundary friction effect decreases. In the case of hexagonal particles, the rotational response of hexagonal particles slightly decreases due to boundary friction. This phenomenon can be attributed to the high rolling resistance and enhanced interlocking features of angular particles. As a result, angular particles tend to have relatively stable edge-wall contacts, leading to significant shear force generation between particle-wall contacts. The shear force generated at the walls contributes to the overall strength of the specimen.



**Figure 7.**  $r_m$  and  $\epsilon_s$  relationship for particles in contact with rigid walls with and without wall friction ( $\sigma_3 = 39.2$  kPa) (a) circle (b) tridecagon (c) hexagon

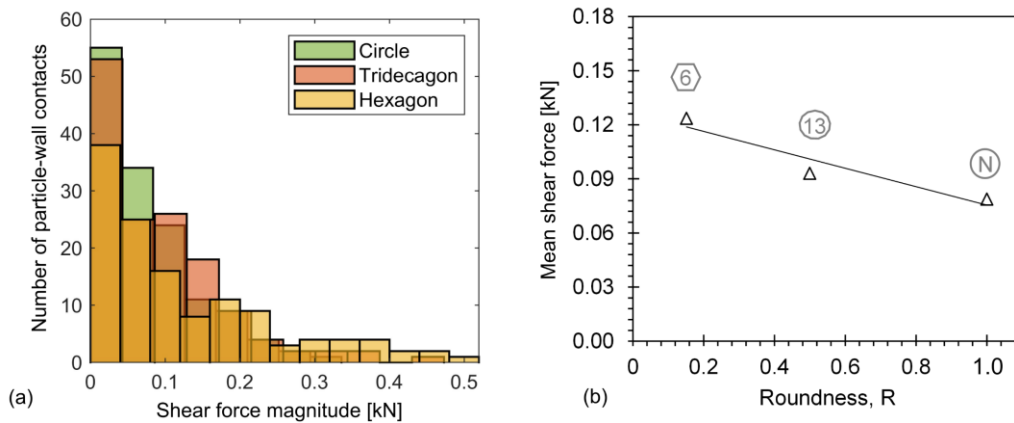
In summary, it can be concluded that angular particles, characterized by their high rolling resistance and interlocking features, can generate relatively higher shear forces at the particle-



wall contact points in the presence of boundary friction. On the other hand, round particles, which lack rolling resistance and interlocking characteristics, tend to rotate much, and prevent significant shear force generation at the particle-wall contact points.

### 3.4 Particle-wall contact shear forces

When a granular sample undergoes deformation due to external loads, forces develop at the contacts between particles. These contact forces can be categorized into normal (compression) and tangential (shear) components. The shear component of contact forces is typically influenced by the frictional properties of the contacting surfaces. Similarly, when a frictional boundary is present, shear forces are also generated between the particles and the boundary. Whether these generated forces contribute to the overall strength of the specimen depends on the shape of the particles. Figure 8a shows the distribution of shear force magnitudes for all RWC particles in the case of frictional boundary simulation under  $\sigma_3 = 39.2$  kPa. It can be seen that the number of particle-wall contacts experiencing significant shear force increases with the increase in the angularity of the particles in contact with frictional walls.



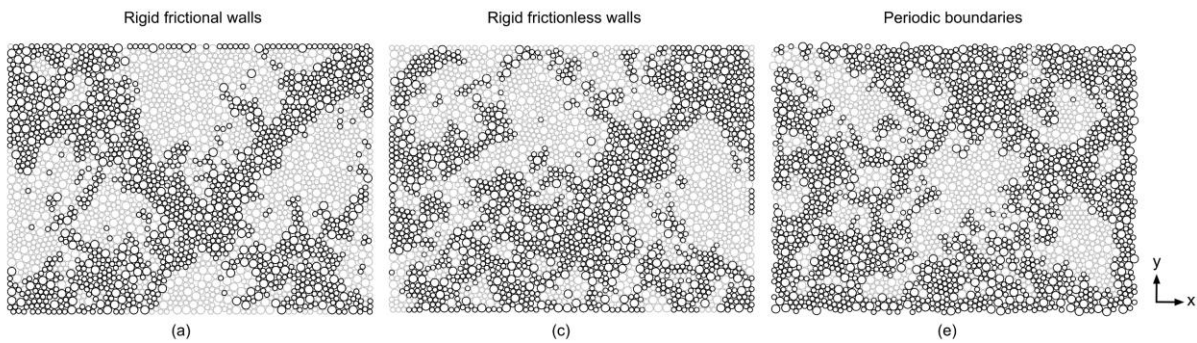
**Figure 8.** (a) Frequency histogram of shear force magnitude (b) average shear force magnitude per particle-wall contact under frictional boundary ( $\sigma_3 = 39.2$  kPa)

Particle shape plays a key role in controlling rolling resistance and interlocking characteristics. Consequently, in the presence of shear forces, RWC circular particles tend to rotate, avoiding the generation of intense shear forces at the boundary. On the other hand, for angular particles, rotation is limited, resulting in relatively significant shear forces at the boundary, which contribute to the overall strength of the specimen. Figure 8b illustrates the average shear force experienced by all RWC particles depicted in Figure 8a. It can be observed that RWC circular particles exhibit the lowest magnitude of average shear force, whereas the magnitude increases with the angularity of the particles. This further emphasizes that RWC round particles can rotate and minimize the influence of boundary friction. On the other hand, RWC angular particles are more significantly affected by boundary friction.

### 3.5 Boundary effecting deformation patterns

When external loads are applied to granular materials, uniform deformation occurs initially. However, as the deformation progresses, the magnitude of deformation becomes concentrated,

resulting in the formation of localized regions known as shear bands [11,23]. The formation of shear bands can be influenced by various factors, including boundary conditions. The microstructural constraints within the shear bands are different therefore, it is crucial to accurately identify and characterize these shear bands in granular samples [21]. This study investigated the impact of boundary conditions on the formation of shear bands. To identify the particles within shear bands, a shear strain criterion was employed, which involved assigning a deviatoric strain value to each particle using a post-processing procedure developed for the DEM by Catalano et al. [24]. The procedure utilized a regular Delaunay triangulation available within the YADE software to identify a Voronoi cell with vertices at the mass centers of the particles [25]. The particle positions at two different instants towards the end of shearing, specifically at deviatoric strain levels of 24% and 30%, were input into YADE. The displacements of neighboring particles were then utilized to compute a strain tensor for the triangular element. Subsequently, the deviatoric strain was assigned back to each particle by averaging the deviatoric strain of the adjoining triangular elements. To identify particles located within the shear band, a threshold deviatoric strain of 5% was applied. Rorato et al. [26] and Ali et al. [20] employed the same technique to assign particles to shear bands in 3D triaxial and 2D biaxial experiments, respectively.



**Figure 9.** Effect of boundary condition on shear band formation (a) rigid frictional walls (b) rigid frictionless walls (c) periodic space, (black outlined particles belong to shear band)

The results of shear band identification for simulations of circular particles with different boundary settings are presented in Figure 9. The choice of boundary setting has a significant impact on the deformation patterns. Figure 9a illustrates that when rigid frictional walls are employed, the deviatoric strains tend to concentrate in two distinct X-shaped zones, aligned prominently along the diagonals of the biaxial box. On the other hand, Figure 9b demonstrates that with rigid frictionless walls, the formation of shear bands becomes more random throughout the biaxial box, and several small isolated microbands can also be observed. In contrast, when periodic boundary settings are utilized as shown in Figure 9c, the random deviatoric strain localization can also be observed. The influence of boundary setting on shear band formation exhibits qualitative similarity regardless of the particle shape.

#### 4 CONCLUSIONS

In this study, we conducted DEM simulations of a biaxial shearing test using polygon-shaped particles with varying numbers of corners, representing different degrees of roundness by

applying different boundary conditions. Firstly, our findings indicate that the effect of particle shape on the mechanical response of granular materials is independent of boundary conditions. This effect is qualitatively similar regardless of the specific boundary settings employed, highlighting the dominant influence of particle shape on the variation in mechanical response. Thus, the impact of particle shape surpasses the influence of boundary conditions.

Secondly, we observed that the choice of boundary setting plays a significant role in simulating the response of granular materials. For a given particle shape, when rigid frictional walls are utilized, the granular materials exhibit relatively maximum shear strength. Conversely, the application of rigid frictionless walls leads to a slight decrease in shear strength, and the relatively minimum strength is observed when periodic boundary settings are employed. The magnitude of the change in shear strength resulting from the change in boundary conditions is closely linked to the shape of the particles. When altering boundary settings, angular particles display a relatively higher variation in shear strength compared to perfectly round particles. This disparity arises from the high rolling resistance and enhanced interlocking characteristics exhibited by angular particles. Therefore, the selection of appropriate boundary conditions should be done cautiously, considering the shape characteristics of the particles implemented in the DEM simulations.

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