

Study the Particle Size Impact on the Mechanical Behaviour of Granular Material by Discrete Element Method

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Granular materials are used in various industries, including pharmaceutical and agriculture, where the material properties of elements have an important impact on their flow behavior. Numerical codes based on the Discrete Element Method (DEM) are decisive for describing the flow of granular material. The DEM could investigate granular materials' macro and micro-mechanical shear behaviors. The commercial software EDEM® based on the DEM was utilized for this purpose. A gravitational disposition for the geometrical arrangement model has been performed in this study to model different particle sizes for a direct, simple shear test (DSST). The results indicated that referring to the size index (SI), a positive correlation occurred with the shear strength, dilation, volumetric strain, a negative correlation with the average particle angular velocity, and a neutral correlation with the coordination number (CN).

Keywords: Discrete element method; Granular material; Particle shape; Simple direct shear test; Size index.

1. INTRODUCTION

Granular material is the primary component in the pharmaceutical and agricultural industries [1]. There are a lot of factors that affect the mechanical behavior of the granular material bed, such as loading properties [2], fouling level [3], distribution of particle size [4], the void ratio [5], normal stress and confining pressure [6]; In addition to the individual particle properties: particle size [7], particle shape [8], and strength [9] have an impact on the mechanical behavior. The key parameters determining the response of granular materials are the angularity and surface texture of the particles [10]. It has been revealed that particle degradation depends on particle shape [11]. Complex-shaped particles are more likely to break than cubic particles; however, in the experimental study, it is challenging to provide a straightforward approach to find the evolution of particle angularity/texture during the shear test due to the costly experiments and the large-scale limitation. Therefore DEM simulations are applied instead to investigate the behavior of granular materials.

Because of the drawbacks mentioned above, DEM models have been developed to study the behavior of granular materials for decades. Moreover, DEM allows analyzing the results achieved by varying the parameters of the simulated materials, particularly the shape index [12]. It was demonstrated in a previous study where authors used two-dimensional simulations that revealed the shear strength, dilatation, and latent shear strength increased as the particles' angularity raised [13]. On the other hand, describing such par-

ticles' actual shape in DEM simulations is still challenging. At the beginning of DEM simulations, the description of a real particle shape could only be modeled using a disk or a sphere [14]. Despite the simple DEM algorithm for detecting the interactions and measuring forces, the actual structure of a particle needs to be modeled because using a regular shape such as a disk or sphere would provide appropriate rolling resistance compared to the original particle shape. When considering particles as disks or spheres, their rotation is solely influenced by the tangential component of the contact force; the moment on such particles has no effect since the normal force is oriented towards the center [15-17]. These techniques have been used in railway research to model ballast particle shapes.

In a previous study, the behavior of a ballast settlement was analyzed through DEM using polygon-shaped elements to mimic the actual shape of the ballast particulates under dynamic loading [18]. Researchers revealed that particles having a size inferior to half of the nominal maximum size of the actual particle are inadequate to conduct a full-scale ballast layers simulation [19]. In another work, a similar approach was utilized when modeling ballast layers [20,21], while another study produced a 2D projection of complex-shaped ballast particles using clusters of bonded circular particles [22]. In conclusion, 3D simulations have been conducted to model ballast similarly [23]. However, ellipsoidal particles [15], elliptical particles with oval-shaped boundaries [24], particles shaped like polygons [25], particles with dense clusters overlapping [16], and particles with axial symmetry may not adequately describe the actual shapes of these particles [26].

Furthermore, a few of these methods need significant computing time. Therefore, to simulate the particle form, researchers presented an approach based on a simple algorithm widely used in DEM; in this procedure, the overlapping spherical components are

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tightly joined, which offers the advantage of modeling a particle shape with varying angularities while following the same contact laws as a single sphere [27]. Modeling the real shape of ballasts has been done using this method. Researchers simulated The geogrid-reinforced ballasts to decide the ideal position for a geogrid [28].

While most numerical studies tackled the modeling of actual particle shapes and the mechanical responses of the ballast layer under different situations, the effects of the particle shape on the mechanical results, which are complex to analyze in laboratory experiments, are cumbersome in the literature. Moreover, due to the minimal friction between particles, scientists conducted a simple direct shear test, proving that when using a fouled particle, the particle's shear strength decreased due to a reduction in the friction angle[29]. They Moreover found that dilation occurs in the fouled ballast sample by applying a high rate of fouled particles, particularly at a low normal stress level. Additionally, employing a geogrid was in prime agreement with DEM simulation and lab data of coal-fouled ballasts [30]. In conclusion, the sleepers' side resistance was reduced using fouling particles in the ballast bed, especially when fouling particles were placed at the edge of the ballast bed [31].

Researchers have studied the random shape and size of the particles in terms of angularity index AI where the AI analyzes the particle in terms of the number and sharpness of the corners [32], and the sphericity index SPH which the SPH represents how closely an object's shape matches a whole complete sphere [33]. Therefore, a new study path has been established by studying particles with a definite shape and size. For instance, this new study path has examined the effect of different SPH for the same definite particle size [34] and different size index SI for a certain shape triple particle, where the SI represents the size variations of a definite particle shape [35]. In addition, the main objective of this study is to examine the effect of double particle size index SI on the particles' mechanical behavior in the direct, simple shear test (DSST).

2. THE DISCRETE ELEMENT METHOD (DEM)

Instead of the conventional cost-effective trial-and-error method, the DEM is an excellent tool for modeling the mechanical properties of bulk material and a whole process of particle blending [36].

The Method of Discrete Elements (DEM) was developed to simulate the mechanical behavior of granular materials. Newton's second law of motion describes the translational and rotational motion of every particle in the DEM system [37,38]. During the simulation circle, The normal and tangential forces generated among particles and between particles and the wall are computed using a calculation loop that involves applying Newtonian equations of motion repeatedly to generate each particle's acceleration, velocity, and displacement values, as described by the following equations [36]:

$$F_t = -8G_0\sqrt{R_0\delta\delta_t} - 2\sqrt{\frac{5}{6}} \frac{\ln C_r}{\sqrt{\ln^2 C_r + \pi^2}} \sqrt{2C_0} \sqrt[4]{R_0\delta} \sqrt{m_0 v_{nrel}} \quad (1)$$

The young E_0 module equivalent of two intermingling particles is derived from the following formula.

$$1/E_0 = (1 - v_1^2)/E_1 + (1 - v_2^2)/E_2 \cdot \delta$$

Represents the amount when those two particles collide, and C_r is the coefficient of restitution (described in EDEM® [39] as the ratio of separation to approach speed in a collision). The normal overlap δ characterizes normal particle deformation.

$$F_t = -8G_0\sqrt{R_0\delta\delta_t} - 2\sqrt{\frac{5}{6}} \frac{\ln C_r}{\sqrt{\ln^2 C_r + \pi^2}} \sqrt{2C_0} \sqrt[4]{R_0\delta} \sqrt{m_0 v_{nrel}} \quad (2)$$

The equivalent shear modulus of two entangled particles G_0 is calculated using the following formula:

$$1/E_0 = (1 - v_1^2)/E_1 + (1 - v_2^2)/E_2 \cdot \delta$$

Describes the tangential overlap of two particles, representing the tangential deformation. Tangent overlap is the tangential movement between two particles from first to last contact, whether when one particle rolls or slips against another. And v_{trel} Is the tangential component of relative particle velocity.

The particles' recent displacement obtained is utilized to further calculate the contact forces and torques in that area of contact due to the particles' interactions in the newfound position. This simulation cycle is applied repeatedly through time to describe the flow of the bulk material [40]. This method is ideal for analyzing the movement of a granular material [41] and examining the vibration effect [40]. Researchers predicted that the DEM models might be used to determine and analyze the pressure distribution in a silo by simplifying the design process for this sort of equipment [42]. DEM Furthermore investigate the flow patterns, segregation, discharge rates, and the effect of flow patterns in silos [40]. The discrete element technique is powerful for illustrating particle motion in various scenarios. Torques are calculated using DEM based on particle displacement in every timestep. The behavior of particles and interactions highly depends on the particles' shape and the different micro-mechanical properties [40]. The commercial software EDEM® was used by adopting the "Hertz Mindlin No-Slip" contact model [39].

3. DEM SIMULATION OF THE SHEAR CYLINDER

The numerical experiments were carried out in a cylinder having a 225 mm height and a 52 mm radius, as illustrated in Figure 1. The lower part of the cylinder has a height of 75 mm and was set to move only horizontally, while the upper part of the 150 mm height is fixed in all directions. The horizontal displacement of the lower part in the DEM model was allowed to move for a distance of 30mm (around 15% of shear strain), which is sufficient to reach the peak of particles' shear stress. The vertical loading test applied a constant normal load on the sample. The horizontal loading test applies a shear force to the sample at a constant displacement rate.

A definite number of particles having similar shapes and sizes were generated in each simulation. Then, the particles were packed into the cylindrical container under the effect of gravity and were allowed to repose until the bed's free-motion state reached. This initial state was considered for all the simulation cases. The simulation scenarios were executed in three stages. Initially, particles were rapidly generated through a factory into the cylinder where the kinetic energy dominates, and a high contact between particles occurred. Afterward, the generated particles require settling time, and null kinetic energy is attained. During the second stage, the material bed was subject to a vertical load by letting a ball with almost the same diameter as the cylinder fall on the particle bed; the ball's adjustable density allows to apply several vertical loads from the top of the DEM system. Furthermore, the spherical shape of the loading tool (ball) helps us avoid the particle bed's locking volume problem during the shear test as it lets the material bed freely move vertically even under loading, which is a common problem during DEM shear tests[43].

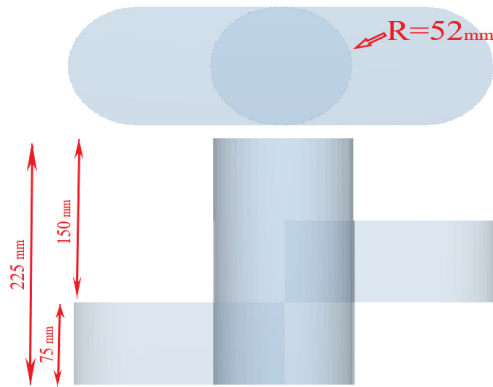


Figure 1 Schematic of model geometry

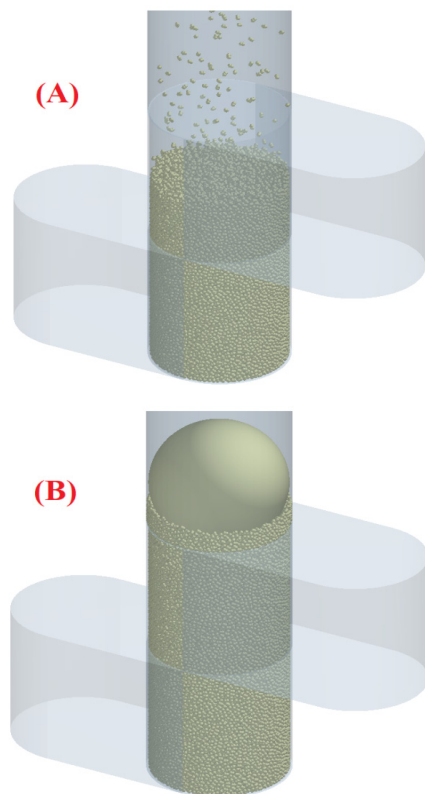


Figure 2 Shear box Simulation and assembled generation Stages particles with a 100% size ratio under 3 kPa normal pressure. (Articles generation, Bcompressed by normal stress, C shearing process)

The final step was accomplished by performing a direct, simple shear test by moving the lower cylinder of the model horizontally while maintaining the vertical load constant during the shear, as illustrated in figure 2.

3.1 Model Parameters

We simulated a large-scale model of the real direct, simple shear test cylinder using a solid wall and a deadweight sphere (ball) above the particles bed in the upper cylinder. This rearrangement allows the particle's volume to fluctuate freely during the shearing process. Figure 3 illustrates a defined SI for a five-particle used during the simulation. (Size Indexes= 50%, 75%, 100%, 125%, 150% for all the particles, respectively). During all the simulations, the particle size for each simulation was the same to minimize the degradation effect. The particle radius and the distance between the centers of the particles vary with each repetition: (R= 0.5mm, 0.75mm, 1mm, 1.25mm, and 1.5mm) as revealed in Fig 3. for each simulation scenario, particles with a particular shape and size were generated. The SI=50% assemblies have 596000 particles, SI=75% assemblies have 280000 particles, SI=100% assemblies have 110000 particles, SI=125% assemblies have 60000 particles, and SI=150% assemblies have 32000 particles. For each run, the normal gravity forces compact the identical SI particles that fill the shear cylinder, which is repeated for each simulation to allow a successful sample comparison.

Table 1. The model Micromechanical parameters.

Parameter	Value
Particles Poisson's ratio	0.4
Wall Poisson's ratio	0.3
Particles Shear modulus (Pa)	3.58×10^8
Wall Shear modulus (Pa)	8×10^8
Coefficient of restitution	0.5
Coefficient of rolling friction	0.01
Particle density (kg/m ³)	1430
Coefficient of interparticle friction	0.5
Coefficient of plane wall-particle friction	0.6

Furthermore, the ratio distance between the clump centers was kept constant (sphericity index=88%) to preserve the same particle shape. Additionally, four different vertical loads were examined for each SI, and

since we have five different SI, the total number of simulations is twenty.

The DEM parameters in Table 1, based on the previous work, were used in our work to achieve accurate results [36,44].

3.2 Particle Shape Generation

A specific SI was considered for each simulation, with a constant SPH to analyze the effect of the SI on the particle's mechanical behavior.

Fig.3 illustrates all particles' SI values used in this study.

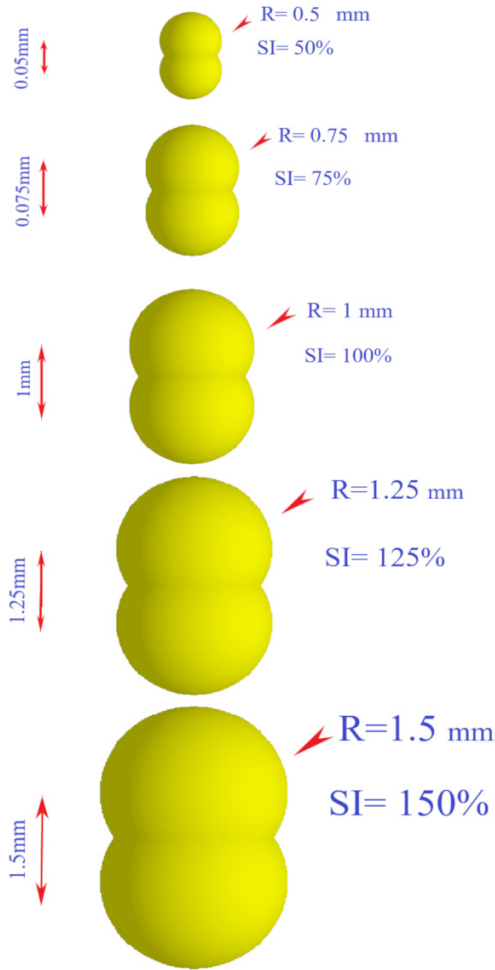


Figure 3. Various particle SI simulations(SI= 50%, 75%, 100%, 125%, 150% for all the particles respectively).

4. RESULTS AND DISCUSSION

This part summarises the particles bed macroscopic and microscopic findings of shear stress, network contact forces, variation of contact number, and average particle rotation in the DSST.

Shear Stress

The forthcoming graphs demonstrate the effect of SI on the relationship between the horizontal strain and the shear stress at a steady rate of normal stress. Furthermore, to calculate the internal friction angle, we measured the arctangent of the shear stress ratio with

the normal stress ratio ($\phi = \arctg(\tau/\sigma)$). Therefore, a positive correlation between the internal friction angle and the particle size is observed with an increase in particle size. The internal friction angle increases with particle size (SI). On the other hand, increasing the SI significantly influenced the findings; two-dimensional elliptical particles had similar outcomes [15]; in addition, 3D ellipsoid multi-sphere assemblies obtained a similar conclusion [45].

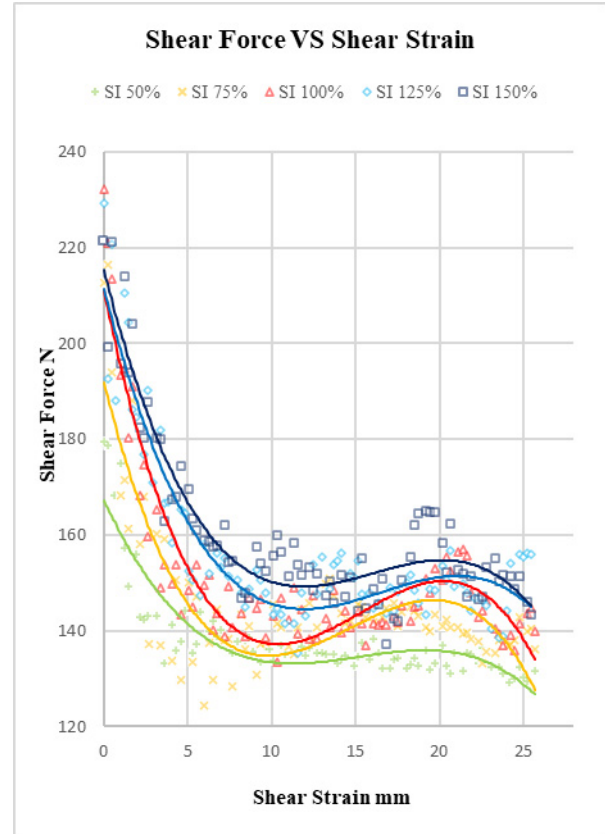


Figure 4 Shear force vs. shear displacement plots of samples with varying SI at 30kPa normal stress

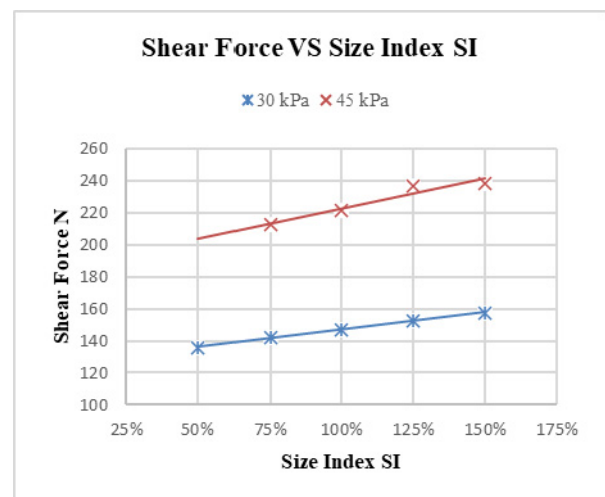


Figure 5 Shear stress with a variety of SI at 30 kPa and 45 kPa normal stress

Comparing particle samples, the influence of the SI is more apparent. This phenomenon illustrates the progression of the moment force and the course interlocking connections between particles under normal stress

(course interaction between the particles). Due to the critical moment required for rotating particles, the large particles would be more frictionally interlocked. For example, at a 30 kPa normal stress, the shear force increased from 136N to 158N when the particle SI changed from 50% to 150%. However, the change in shear force was decreased for smaller SI particles and vice versa.

Fig. 4 is plotted to understand better the effects of the SI on the particles' shear behavior under constant normal stress.

Fig. 5 illustrates that the interlocking particles can be dilated as the normal stress decreases, decreasing the total shear force. When the rate increases, the particle encounters a more effective interlocking rate, gradually increasing the shear stress. In contrast, due to the high normal stress, these particles would not move easily against each other, leading to anisotropy; therefore, the Friction angle is reduced in a sample with less anisotropy [46].

A rise in the shear stress occurs simultaneously with an increase in the SI. For example, in the case of 30 kPa normal stress, when the particles' SI increases from 50% to 150%, the shear force increases by around 15%.

Volumetric Strain

Fig. 6 illustrates the volumetric strain variation with a horizontal strain under different normal stresses. A reverse correlation occurs between the overall volumetric strain and the normal stress; as the normal stress increases, the overall volumetric strain decrease and vice-versa. From this relationship, a lower dilation of particle volume strain occurs under a higher value of normal stress.

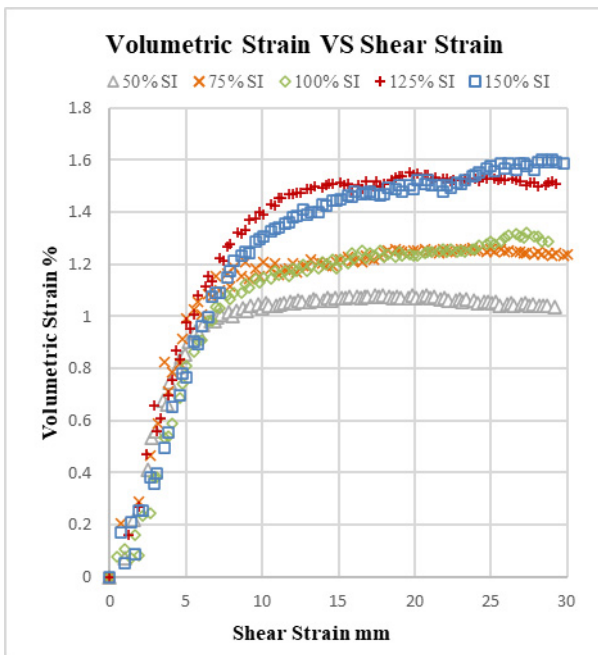


Figure 6 Variations of volumetric strain with shear strain for various normal stresses (SI 150%) Normal stress 30kPa, 45kPa, 60kPa

Fig. 7 illustrates that as the particle's SI increases, the particle volume dilation increase; therefore, it is

clear that the particles' volume dilation depends on the particles' shape and the normal stress[34].

Fig.8 illustrates that a lower level of dilation occurs at higher normal stresses. For example, in the case of a 30 kPa normal stress, The dilation value increase by 28% when the assembly particles' SI change from 50% to 150%.

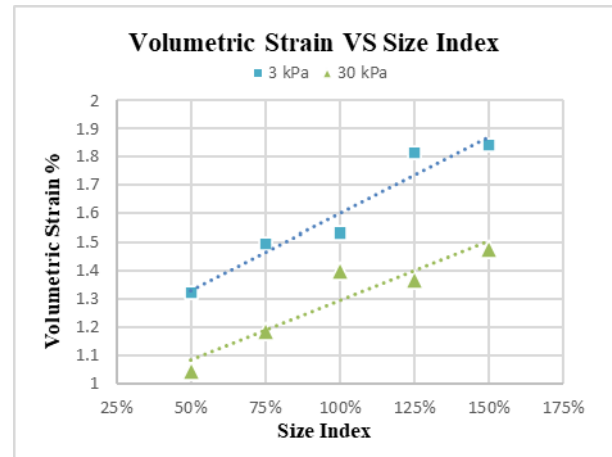


Figure 7 Variations of volumetric strain with shear strain for different size indexes at normal pressure of 30 kPa

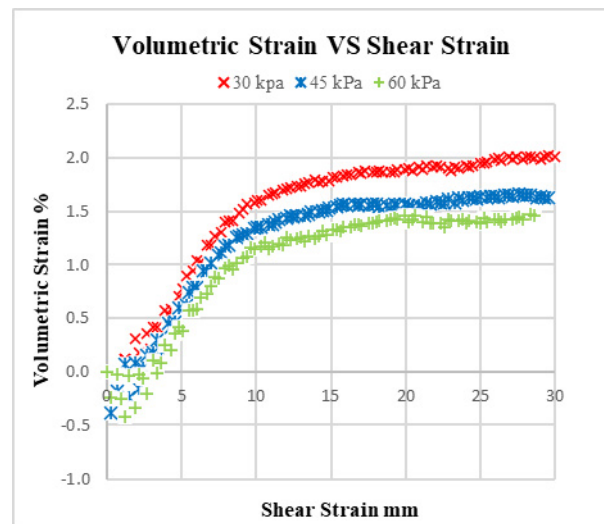


Figure 8 Volumetric strain for different size index values at a normal stress of 3 and 30kPa

4.3 Average Contact Numbers

Particle-to-particle contact ratio, or the coordination number (CN), where CN is the number of particles in contact with the total number of particles in the assembly, CN is a suitable parameter for describing granular materials' behavior since the particle interaction is related to points of contact[32].

As demonstrated in Fig.9, The CN is constant as the SI increases or decreases; the CN remains relatively constant when the SI changes. Therefore, it can be clarified that by increasing or decreasing the SI, the changes in particle shape happen in three dimensions, which means the particle size will change, but the particle shape will be preserved. Therefore, the density of the particle connections in the assembly will stay relatively constant since the SI change does not interfere with the sphericity of the particle. Thus, the sphericity

index will remain constant. Furthermore, researchers mentioned that in the case of changing the particle SPH, the particle shape changes in one dimension, making the particle more elongated, leading to increases in the interlocking between the particles; by giving other particles the chance to have contact with the same particle. In summary, increasing the CN[34].

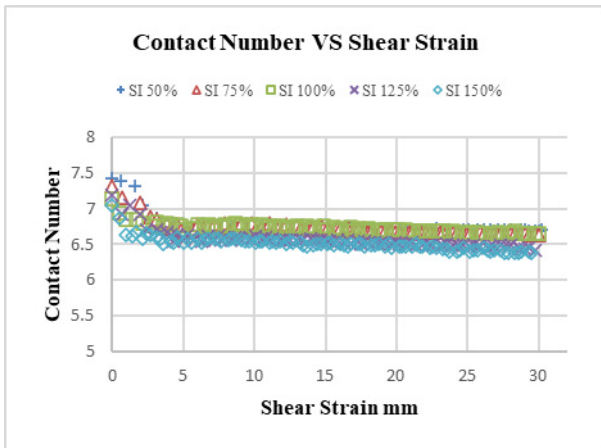


Figure 9 Variations of CN versus shear strain for normal stress of 30kPa (SI effect)

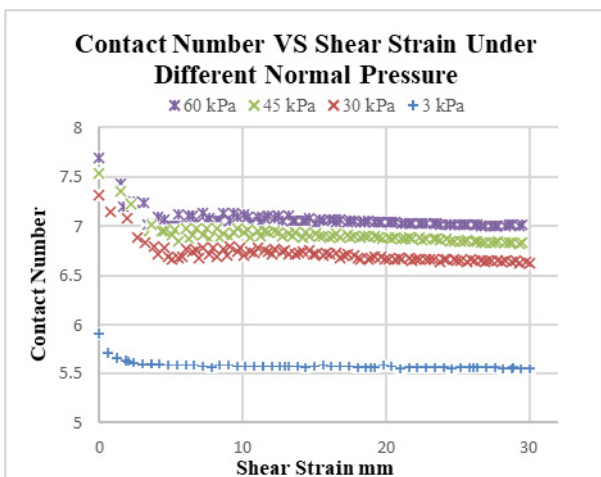


Figure 10 Variations of CN versus shear strain for various normal stresses (SI 150%)

Fig.10 illustrates that a more significant CN was produced, independently of the SI index, when high pressure was applied to the sample. However, A drop in CN is immediately seen in lower normal stress levels due to dilatation caused by the first strain.

The Chain of Contact Force

Figures 11&12 illustrate the forces distribution in the model at different steps of the DSST, where the inter-particle and particle-wall forces are examined at different SI values and normal stresses. These figures also demonstrate the number of contact forces in the model, where the higher contact forces are represented in red, the moderate forces in green, and the low forces in blue. Before the first step by moving the lower cylinder and applying the shear stress (strain 0%), the particles in the model revealed a uniform distribution for all of the models with different particles' SI. However, contact force chain variations are noticeably

different at a 15% strain than at a 0% strain when applied shear force. Fig.11 illustrates a thicker contact forces chain in the first stage of the simulation (0% strain) compared to Fig. 12, which demonstrates the simulation's second step (15% strain). The thicker contact forces are observed because of the dilation behavior of the particles during the shear, causing a decrease in the CN of the particles.

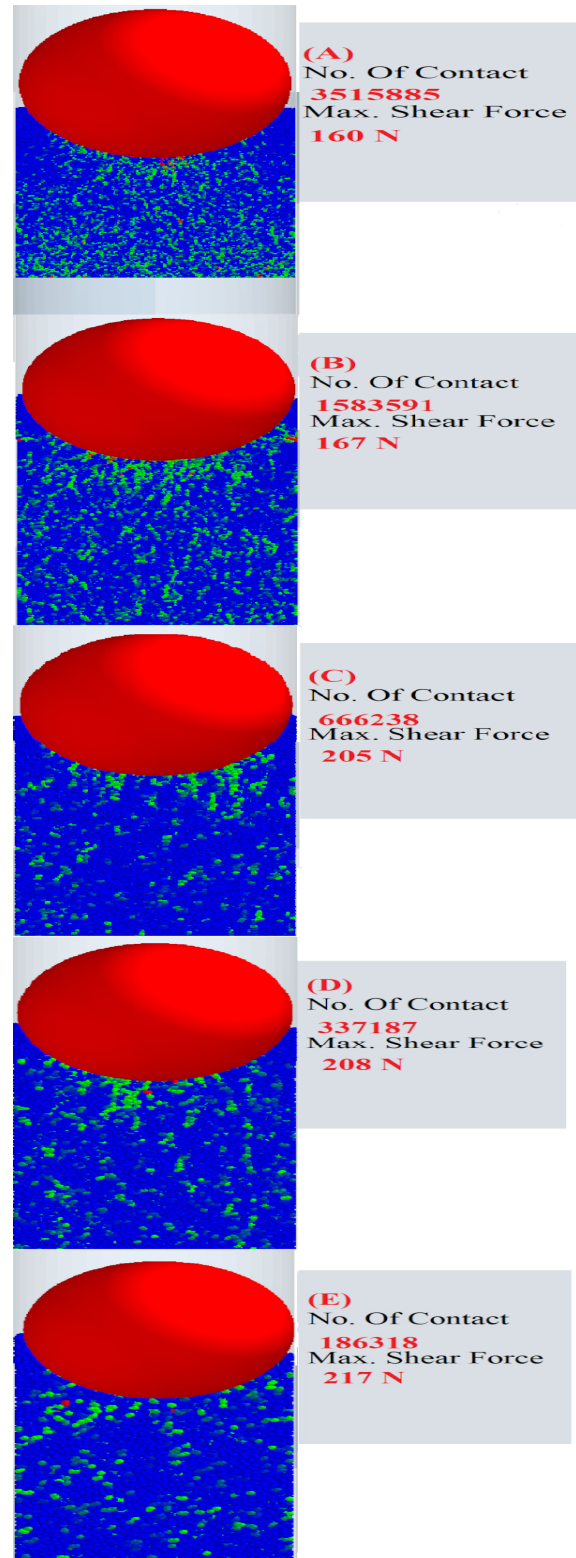


Figure 11 Distribution of contact force chains for various SI particles at shear strain of 0% and 30kPa normal stress (Size index SI= 50%, 75%, 100%, 125%, 150% respectively)

It can be observed from the shear stage that the particles' CN follow the direction of the higher loads (i.e., shear direction). As the shearing is applied to the model by moving the lower cylinder, it causes a reduction in the interaction cross-section area between the two cylinders, resulting in a gradual decrease in the shear stress.

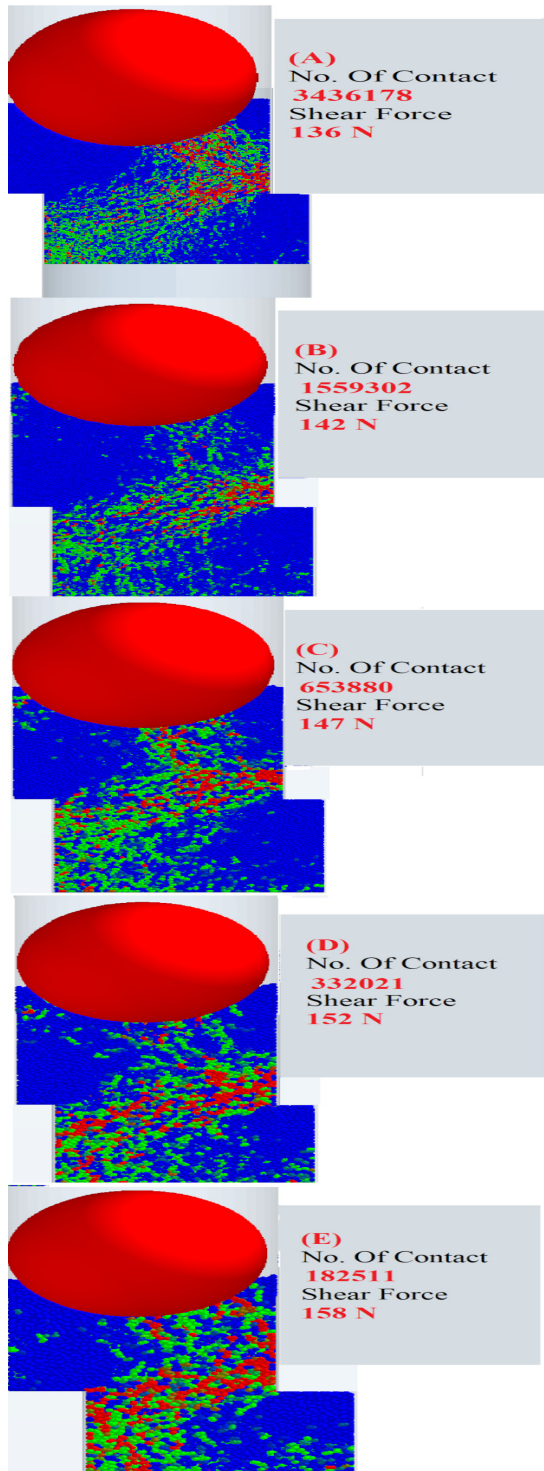


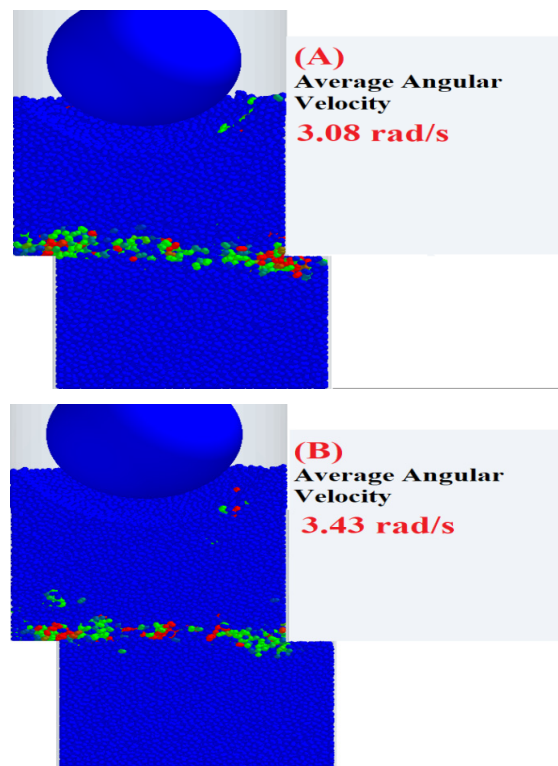
Figure 12 Distribution of contact force chains for various SIparticles at shear strain of 15% and 30kPa normal stress (Size index SI= 50%, 75%, 100%, 125%, 150% respectively)

Furthermore, the sample with a high SI value increases the shear force during the shear stage because of the higher coarse interaction (i.e., better interlocking) as the particles' SI increases. In addition, a study has

similar results, which addressed higher force chains that shaped a greater particle contact in higher SI samples [47]. These circumstances of the mobile part, where the lower cylinder start to move in the right direction to apply the shearing stress, causes the shear band to form from the bottom left of the lower cylinder to the top right of the upper cylinder and hold the most of the load transmission in the assembly. As a result, a stable force chain structure formed. Simultaneously, any particle outside of the shearing band is not participating in carrying the load, as illustrated in Fig. 12.

Shear zone and particle rotation

During the shear process, the rearrangement of the shear band can be estimated by reading the average particle rotation [48,49]. As long as the DSST can be used to evaluate the shear band, studying the particle SI effect on the shear band line and the average angular velocity in the model has been considered in this paper. Fig. 13 illustrates the effect of the SI on the particle rotation in the case of a 15% strain under 30 kPa normal stress, the rotation of the particle can be visualized by using a color code illustrating the particles rotation intensity, where the higher rotational particles are shown in a red, medium in green and low rotation particles in blue. Fig. 13 demonstrates that a higher particle rotation occurs for a large and small particle, and the total average rotation for the large particle's SI=150% is lower than the small particle's SI=50%. Figures 13 & 14 illustrate that interlocking particles increase, and the particle average rotation decreases when the SI increases. For instance, as the shape of the particle increases from SI=50% to SI=150%, the total average particle rotation decrease by 66%. Fig. 14 illustrates the average angular velocity for all SI particles. In conclusion, a positive correlation between the shear strength and SI and a negative correlation between the SI and particle rotation [32].



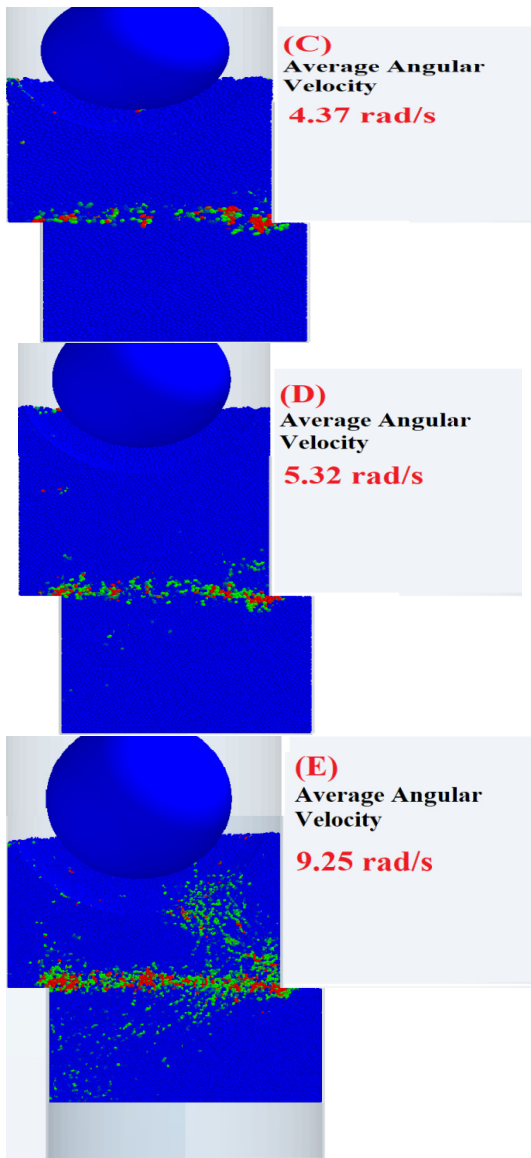


Figure 13 Rotation of particles at 15% shear strain for (SI= 150%, 125%, 100%, 75%, 50% respectively) at 30kPa normal stress

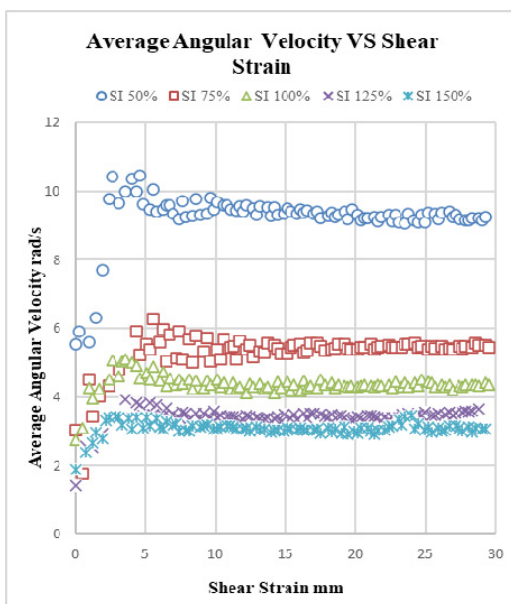


Figure 14 Average angular velocity for different size index particles under 30kPa normal stress

Fig. 15 illustrates the particle's motion behavior, which is described as a movement of horizontal parallel layers, and two factors influence this movement; The normal force begins with, which influences the interlocking between the particles by increasing the friction between them due to better locking. Therefore the rotation interaction will be increased. In addition, the particle shape where the particle shapes impact the friction intensity among the particles. It can be observed that the particles' rotational patterns follow the direction of the shear band, where the particles with high intense rotation tend to rotate along with the shear band direction.

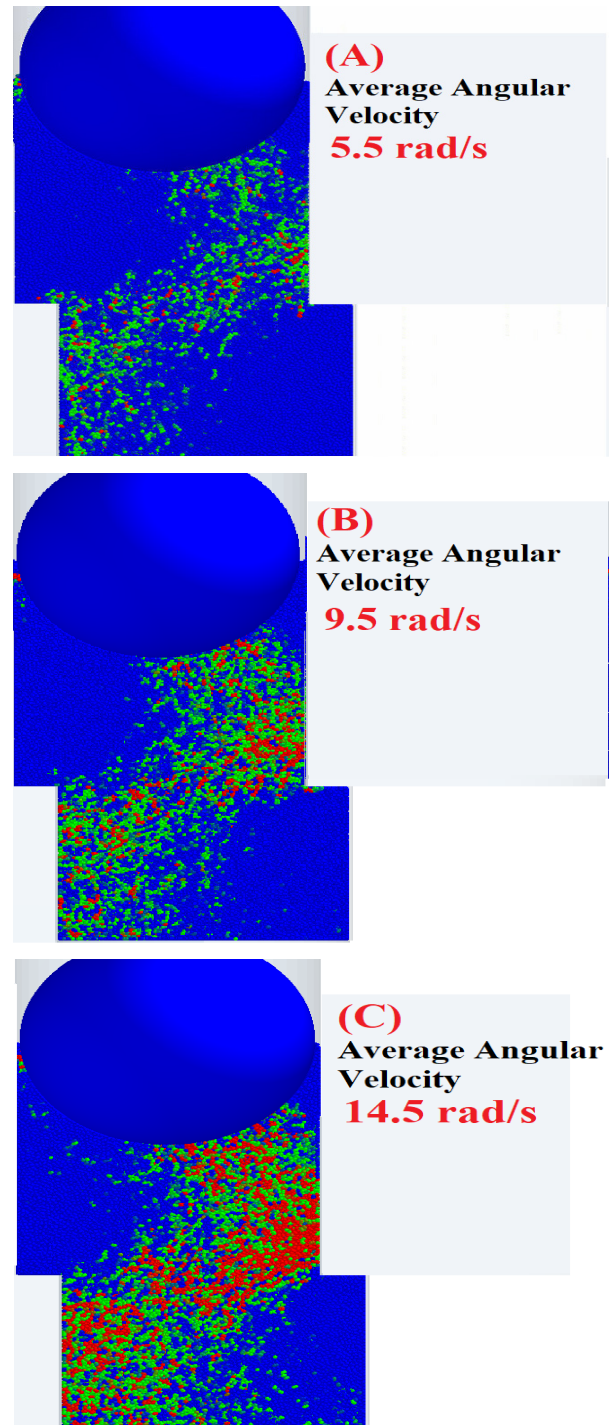


Figure 15 Particle rotation at a shear strain of 15% for a test of SI 75% at different normal stress= 30 kPa, 45 kPa, and 60 kPa, respectively

5. CONCLUSION

This numerical study investigates the effect of particle size on the flow of the bulk granular material. Five particles with different were considered and tested under different normal loads, where the index ranged between 50% to 150% of the particle's actual size. EDEM(3D DEM program)is used to create the particles' shape for a DSST.

The following are the key findings from the examination of both macro-and micro-mechanical properties:

1. Regardless of particle shape, dilation decreases with increasing normal stress in all samples.
2. A positive correlation has been observed between the SI and the particles dilation; however, once the model is subject to a high normal load, the influence of the SI on the dilation becomes insignificant.
3. A positive correlation between the SI and the shear strength has been observed, where the lowest shear strength occurs at the lowest SI value.
4. It does not affect the CN value, and the CN is consistent with the dilation behavior of the assemblies. A reduction in the CN accompanies increased dilation.
5. The size index SI does not affect the CN value because the SI is not influencing the particles' number of contact within the assembly.
6. As the normal stress increases, the CN Increasing due to better particle interlocking.
7. The movement of horizontal parallel layers describes the motion behavior of the particles.
8. At the beginning of the shearing stage, the inter-particle forces are uniformly distributed in all assemblies, then the particles CNis relocated with the shear band direction.
9. The average particle rotation is higher for small-sized particles than for large-sized particles due to less particle dilation.
10. The difference significantly influences the particle's micro and macro mechanical behavior of the DSST.

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**ИСПИТИВАЊЕ УТИЦАЈА ВЕЛИЧИНЕ
ЧЕСТИЦА НА МЕХАНИЧКО ПОНАШАЊЕ
ГРАНУЛАРНОГ МАТЕРИЈАЛА МЕТОДОМ
ДИСКРЕТНИХ ЕЛЕМЕНАТА**

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Гранулирани материјали се користе у различитим индустријама, укључујући фармацеутску и пољопривредну, где својства материјала елемената имају важан утицај на њихово течење. Нумерички кодови засновани на методи дискретних елемената (ДЕМ) су одлучујући за описивање тока зрнастог материјала. ДЕМ би могао да истражује макро и микромеханичко понашање зрнастих материјала на смицање. У ту сврху је коришћен комерцијални софтвер ЕДЕМ® заснован на ДЕМ-у.

Гравитациона диспозиција за модел геометријског распореда изведена је у овој студији да би се моделовале различите величине честица за директан, једноставан тест смицања (ДССТ). Резултати су показали да се у односу на индекс величине (СИ) јавља позитивна корелација са смичном чврстоћом, дилатацијом, волуметријском деформацијом, негативна корелација са просечном угаоном брзином честице и неутрална корелација са координационим бројем (ЦН).