PACKING OF CYLINDRICAL PARTICLE MIXTURES

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Declaration

I hereby, declare that this manuscript, entitled “Packing of cylindrical particle mixtures”, is the result of my own work except for quotations and citations which have been duly acknowledged.

I also declare that, to the best of my knowledge and belief, it has not been previously or concurrently submitted, in whole or in part, for any other degree or diploma at Nazarbayev University or any other national or international institution.

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Date: 7 April 2023

Abstract

Particle packing is significant in manufacturing and chemical engineering. Packing densification by vibration is an important process that affects product storage, transportation, and processing. However, most previous research has focused on the vibrational packing of binary mixtures of spherical particles, while a large part of the powders used in everyday life and industrial production have a non-spherical shape. Therefore, this work aims to study the influence of the shape of the cylindrical particles on the packing structure of binary mixtures and the effect of vibration conditions on packing density.

Packings of binary mixtures of cylindrical particles with different aspect ratios and volume fractions were generated under gravity. In the first part of the study, the impact of the aspect ratio and volume fraction of cylindrical particles on the packing microstructure was studied. The findings demonstrate that mixtures with particles with a high aspect ratio and mixtures with a high percentage of elongated cylindrical particles produce less dense packings.

The intensity of vibration alone cannot adequately characterize the influence of vibration on the packing structure. The second part of the research work was prioritized to consider the impact of vibration amplitude and frequency on the packing density of the mixture. The amplitude range varied between 0.004-0.012 m at a constant frequency of 50 rad/s, and the frequency was between 50-150 rad/s at a constant amplitude of 0.006 m.

The total packing density of three mixtures was calculated for each vibrational condition. As a result, the densification was obtained for the binary mixture with the volume fraction of 50:50 at conditions A=0.006 m, ω= 50 rad/s. With the increase of amplitude and frequency, particles of mixture over-exited leading to a loose packing structure. It was not possible to reach the densification at given vibration conditions for binary mixtures with volume fractions of 25:75 and 75:25. This is explained by the change in particle orientation. To confirm that, a histogram of the angle between the horizontal plane and the particle axes was demonstrated. It was found that after applying vibrational forces particles change their position and tend to orientate vertically, which creates voids and lower packing density.

To study the impact of aspect ratio and volume fraction of the cylindrical particles and the influence of vibration conditions on binary mixtures in more detail packing

fractions of mixtures were analyzed by the voxelization method. The planar packing fraction curves reveal that the lowest packing fraction is produced by a mixture of 75% elongated particles and 25% cylinders with AR=1. Packing fraction along the x and y directions demonstrated the displacement of the particles to one side of the wall at high vibration amplitude or frequency leading to an increase in bed height and a decrease in the packing density. The vibration amplitude and frequency do not significantly change the packing fraction of bottom particles, while top particles over-excite, forming loose packing.

In conclusion, the microstructure of binary mixtures of cylindrical particles with different volume fractions and aspect ratios was studied. The packing density of mixtures was analyzed at different vibration conditions. According to the simulation results, the percentage of elongated particles in a binary mixture can influence the packing structure and the vibration amplitude and frequency can significantly affect the packing density of binary cylindrical particle mixtures by changing the orientation of cylindrical particles in the packing.

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List of Abbreviations

DEM – Discrete Element Method

SQ – superquadrics

MS – multispheres

RDF – radial distribution function

CN – coordination number

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1. Boribayeva, A., Iniyatova, G., Uringaliyeva, A., & Golman, B. (2021). Porous structure of cylindrical particle compacts. *Micromachines, 12*(12). https://doi.org/10.3390/mi12121498.
2. Iniyatova, G., Yermukhambetova, A., Boribayeva, A., & Golman, B. (2022). Approximate Packing of Binary Mixtures of Cylindrical Particles. *Micromachines*, *14*(1), 36. https://doi.org/10.3390/mi14010036

Chapter 1 – Introduction

1.1 General

Improving material qualities is a unique need in chemical and materials engineering in the current world in order to create better goods for human use. Particle packing plays a significant role in various fields, including materials science, pharmaceuticals, chemical engineering, geology and food processing, because it has a substantial influence on the performance of the final product [1]. A variety of parameters, such as packing technique, container shape/boundary conditions, and particle characteristics, can influence packing structure. One of the most essential particle features has been identified as particle shape.

Numerous efforts have been made to study the packing of non-spherical particles. One of the key tasks in the study of the non-spherical packing of particles is to improve the material properties. For example, in the pharmaceutical industry, powder packaging can have a significant impact on the dissolution rate and bioavailability of a drug [2]. Packaging of non-spherical particles in materials science can affect such mechanical qualities as strength and fracture toughness [3]. Similarly, in food processing, the packaging of powders and grains can determine the texture and fluidity of the final product [4].

The researchers mainly focused on the study of binary mixtures in order to improve the packing density of non-spherical particles. Previous studies have focused on the packing densification of binary spherocylinders [5] and binary cylinders [6]. There is still a need to systematically carry out additional work on studying non-spherical particles using numerical analysis to evaluate their packaging characteristics

To sum up, there is a need to investigate the influence of the particle shape and external forces on packing density.

1.2 Aim and objectives

As a result, the objective of this work is to study the microstructural characteristics of cylindrical particle mixture compacts. To that purpose, research will be concentrated on:

1) modeling binary cylindrical particles mixtures by varying aspect ratio and volume fraction and applying vibrational forces using the Discrete Element Method;

2) characterizing influence of the aspect ratio and volume fraction on packing structure of binary cylindrical particle mixtures; and
3) investigating the effect of vibration parameters on the binary mixture compacts.

1.3 Thesis layout

The following sections comprise the thesis organization: Chapter 2 is devoted to a study of the literature on alternative approaches for particle compact packing and non-spherical shape formation utilizing the Discrete Element Method (DEM), application of vibration parameters and voxelization-based packing fraction analysis; in Chapter 3, methodologies were developed for generation of packing samples of poured and vibrated binary mixtures of cylindrical particles, and the procedures of voxelization based analysis to estimate packing structure; Chapter 4 examines results and discussion parts of work estimating packing structure analysis; lastly, in Chapter 5, considers to the achieved results and recommendations for future study.

1.4 Contribution

The principal contributions of the author are:

- Generation of packings of binary cylindrical particle mixtures using Aspherix-GUI software.
- Studying total packing density, particle orientation and distribution of local packing fraction.

Chapter 2 – Literature Review

2.1 Particle packing

Particle packing is significant in both nature and industry. In various sectors, proper particle packing structure is critical to several industrial processes starting from advanced material production to raw material preparation. A variety of parameters, such as packing technique, vessel boundary/shape conditions, and particle characteristics, can influence packing structure. Understanding the characteristics controlling particle packing is critical for achieving the densest packing, which can minimize invading space while increasing the strength of bulk granular material.

The packing of uniformly sized spherical particles has been the most extensively researched subject in particle packing. Cylindrical particles, on the other hand, are widely used in industry. Many materials, such as wood, plastic, herbicide, insecticide, fertilizer, and pet food, are pelletized in the shape of cylinders. Packings of non-spherical particle simulations have lately been examined due to the considerable influence of particle shape on the packing properties of materials. Previous works focused on studying the effect of aspect ratio on the packing structure of cylindrical [7] and spherocylindrical [8] particles at both microscopic and macroscopic levels.

In order to enhance the packing density of irregular-sized particles, scientists focused on binary mixtures. Some studies have concentrated on the packing densification of binary spherocylinders [5] and binary cylinders [6] performed by computer simulation, the latter to verify the model. Liu et al. [9] studied the packing properties of binary mixtures composed of superballs and spheres with different size ratios and documented the properties of superballs of equivalent packing sizes, concluding that the unmixed particles are packed denser than binary mixtures and that a larger vessel is required to pack the mixtures of particles. There have been fewer systematic works on the packing densification of binary cylindrical particle mixtures.

To summarize, the study of binary mixtures of non-spherical shaped particles is a current topical concern for packing structure examination that has significantly improved the interest of many researchers in powder technology and chemical engineering. Therefore, this study aims at developing the topic of a binary mixture of irregular-shaped particle packing.

2.2 Packing densification

Packing densification is an important characteristic in industries such as agriculture, food, and mining because it influences product storage, shipping, and processing. The packing characteristics of cylindrical particles differ from that of spherical particles due to the geometry and orientational anisotropy containing different kinds of surface elements [10], making it unrealistic to study the packing densification of cylindrical particles using spherical particle packing models. Non-spherical particles pose a challenge in achieving high packing densities, as their shapes do not allow them to pack efficiently. Physical experimental research on packing densification is generally limited because micro features such as radial distribution function (RDF), coordination number (CN), contact types, particle orientation and contact forces, and orientation distributions in packings are challenging to measure. The experimental findings show [11] that the suggested analytical model is effective in estimating cylinder random packing density. Various analytical and numerical models were proposed to examine the packing densification of cylindrical particles for this aim [12]. One approach to increase packing density is to apply external forces, such as vibration, to the system. Wang et al. [13] systematically studied the influence of the vibration amplitude, vibration frequency and vessel size on the packing density and showed that vibration amplitude, as compared to vibration frequency, is more important for densification since a wide range of acceptable amplitudes are available to produce dense packing arrangements. According to Gan et al. [14], one-dimensional vibration leads to increased packing density for ellipsoids with varying aspect ratios. In another respect, Yogi et al. [15] investigated the segregation and mixing of irregular-shaped particles in a vibrated packed-bed mixer and chose certain bidisperse mixtures to investigate the effect of different parameters.

Several variables, such as vibration condition, particle characteristics, and particle properties, influence vibratory packings. The intensity of vibration cannot fully describe the influence of vibration on packing density. Denser packing requires consideration of vibration amplitude and frequency. An et al. [16] demonstrated 3D vibration packing of uniform spheres and revealed that if the vibration amplitude or frequency is too strong, particles are over-excited, resulting in loose packing. Understanding these effects is crucial for utilizing knowledge not just in fundamental research but also in technological applications. Similarly, Salamat et al. [17] investigated the horizontal vibrating packing of spherical mixtures and specified the vibration frequency and amplitude values required to achieve the greatest packing density.

Physical experiments on packing densification of cylindrical [12] and ellipsoidal [18] particles under mechanical vibration revealed that the packing density first increases to a maximum and then decreases with increasing vibration parameters. A similar characteristic is found for binary mixtures of cylindrical particles. In the study of An et al. [19] physical experiment for packing densification of binary cylindrical particle mixtures under 3D vibration was conducted. The results showed that the packing density of the binary mixture increases with an increase in the size ratio. Under constant vibration conditions, the packing density of each binary mixture of cylindrical particles first increases with an increase in the volume fraction of large particles to a maximum and then decreases. The packing of cylinder mixtures with varied aspect ratios has previously been researched in the literature, but less attention has been made to the packings densified by vibrations.

According to a review of the literature, an analytical model is an effective way to predict the packing density of binary cylinders with different volume fractions and aspect ratios under vibrational forces. The effects of vibration frequency and amplitude depend on the particle shape. Further studies are needed to investigate the effects of vibration conditions on the packing of non-spherical particle mixtures.

2.3 DEM simulation

Theoretical studies have been developed progressively in recent years as computer capacity has improved, and thus its applications have attracted many scientists. Computer power has demonstrated tremendous potential in numerous areas, particularly the advancement of computational engineering materials science. The different kinds of numerical analyzes available can help to broaden our knowledge and understanding of material characteristics.

Despite breakthroughs in supercomputer technology, simulations are still limiting in their ability to simulate increasingly complicated bodies and assemblies. The simulation of numerous complicated processes is one of the major obstacles, and only a few technologies can reach this purpose. The Discrete Element Method (DEM) is a numerical approach for modeling particulate/discontinuous material behavior. Its key components include contact detection, force-displacement relations, friction, Newton's equations of motion, and a time integration mechanism to update particle locations at consecutive time steps [20]. DEM has been used to investigate different aspects based on the discreteness of complex systems like powder materials. In one of the previous research publications, it was proposed to use DEM as a powerful instrument to analyze particle packing in order to increase the efficacy of construction materials. Wu et al. [21] approved the notion of using numerical analysis to achieve available volume maximum packing in the context of lowering concrete environmental impact.

The improved DEM approach has introduced new ways to construct non-spherical shapes, such as multispherical (MS) and superquadrics (SQ) in the literature [22]. The MS approach employs overlapping spherical particles to construct particles of chosen shape, whereas the SQ method uses superquadrics to create particles with rounded or sharp corners. Soltanbeigi et al. [22] demonstrated the increased capabilities of both MS and SQ approaches for the creation of irregular-shaped particles. Non-spherical shaped particles had better packing, as predicted. As the SQ method is more cost-efficient and simpler than the MS method in this research SQ approach will be applied to generate cylindrical particles.

There have been several works on DEM modeling of cylindrical particle packing. For example, Doraia et al. [23] employed the Grains 3D DEM to simulate the poured packing of cylinders in cylindrical tubes. They looked at average porosity, pellet orientation, radial porosity, and the fluctuation of those measures as they repeated the numerical trials. Using the DEM, Hao et al. [24] simulated various size distributions of cylindrical particle shear flows caused by friction. The impact of particle size distribution on the jamming volume fractions of polydisperse flows with frictional cylindrical particles was explored.

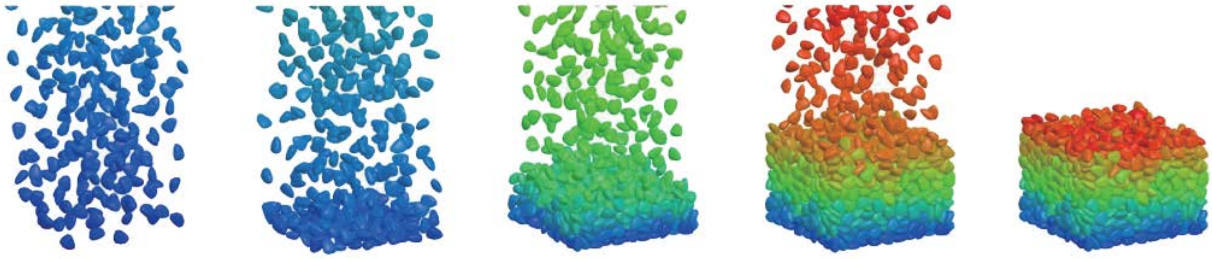


Figure 2.1: Packing process of non-spherical particles *[25]*

Nan et al.[26] employed DEM to generate random loose packing of curl indices with varying aspect ratios (0.03-0.4) and fibers (5-50). Packing porosity, coordination number (CN), contact orientation, and fiber orientation were used to describe the packing structures.

Recently, we proposed the concept of analysis of the packing structure of binary mixtures of cylindrical particles with different aspect ratios using DEM [27]. The simulation results showed that particle aspect ratio and volume fraction have an impact on packing structure.

Apparently, one benefit of DEM simulation is that it may offer microscopic information such as contact force networks and stresses that cannot be acquired through physical tests or Monte Carlo based simulations, but related research in this area is currently scarce. Moreover, the aforementioned experiments were mostly limited to spherocylinder packings, and the ARs were often greater than 1. As a result, it is critical to explore the random dense (or close) packings of various shaped cylinders using DEM.

Less work was done on the packing densification of cylindrical particle mixtures using DEM modeling. Particular attention must be paid to the numerical implementation of close or random dense packing under mechanical vibration, as well as the associated macro/micro property characterization, including contact types, local structures, stresses, forces, and so on.

2.4 Superquadrics

Irregular-shaped particles can be idealized to some regular shapes like cuboids, spheroids, or cylinders, which can be modeled by superquadric (SQ) approach [28], [29]. According to Barr [30], superquadric can be described:

$$f(x,y,z) = \left(\left|\frac{x}{a}\right|^{n_2} + \left|\frac{y}{b}\right|^{n_2}\right)^{\frac{n_1}{n_2}} + \left|\frac{z}{c}\right|^{n_1} - 1 = 0, \tag{1.1}$$

where a, b, c are half-lengths in coordinates x, y, z. The shape sharpness parameter n_1 defines the shape of the cross-sections in the y-z and x-z planes, and the parameter n_2 defines the shape of the cross-section in the x-y plane.

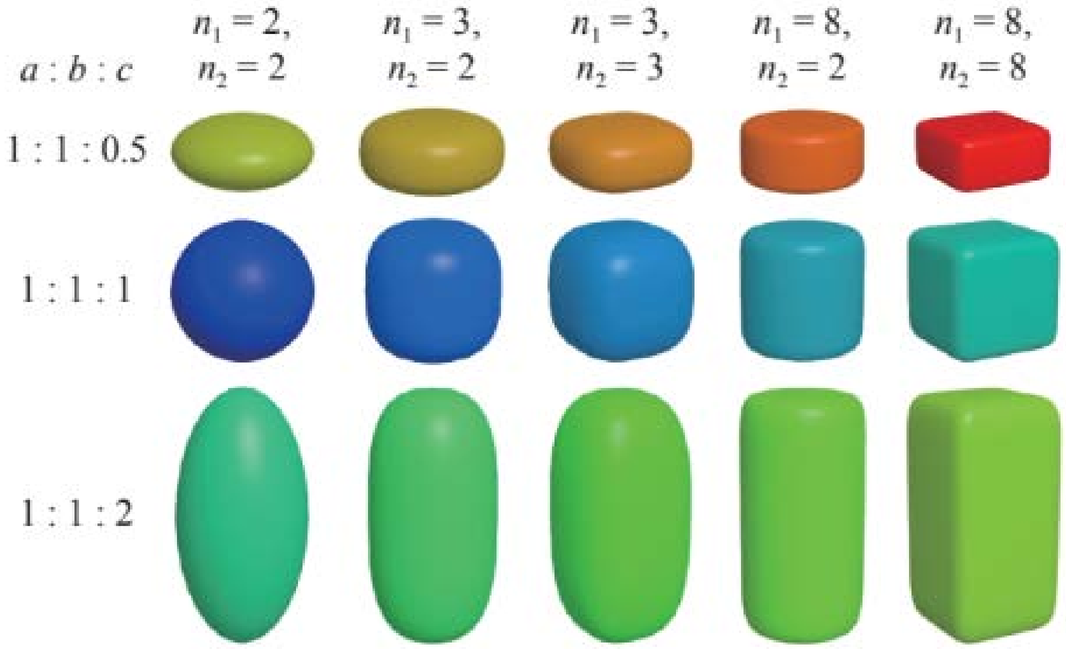


Figure 2.2: Differently shaped particles modeled by superquadric equations** [25]**.

It has been suggested that superquadric functions can represent 80% of all forms or can be generated from superquadrics in higher-dimensional hyperquadrics [31]. SQ particles offer an outstanding balance of model complexity and form variety. With only five shape parameters changed a spherical particle may be transformed into a cylindrical, ellipsoidal, or box-like particle (Figure 2.2). These particle morphologies may capture numerous physical properties of actual compacts, extending the spectrum of DEM application. Pereira & Cleary [32] investigated the segregation of binary mixture constituted of cubes represented as spheres and SQ in a gradually rotating cylindrical tumbler. Scientists observed that the spherical particles segregate to the curved sides of the tumbler, whereas cubical particles segregate to the inner core of the particle bed. It was discovered that spherical particles save more energy than blocky particles and so move faster over the free surface.

In conclusion, it was discovered that superquadric is useful for representing irregular forms of practical powder compacts. Knowing about the characteristics of irregular-shaped particles contributes to the application of superquadric shapes in terms of their attributes and the development of desired forms. In this thesis superquadrics approach has been applied to generate non-spherical particles and reciprocal packing

2.5 Voxelization based analysis

Particle packing is affected by factors such as particle size distribution [33], the presence of walls [34], vibration, different loading conditions [35], particle shape [36], and so on. The only way to study these effects is to discover how packing density changes over the domain. Individual effects of the aforementioned components cannot be recorded and studied using the average packing density [37]. One way to characterize assembly packing variation is to calculate the variance of the packing fraction in each given direction. Calculating the planar packing fraction on closely spaced planes in the desired direction may be used to show how the packing varies along the plane. The planar packing fraction is the ratio of the plane's entire area to the sum of the geometries imprinted on it by the particles. A few studies on the packing fraction variation for spherical particles have been conducted [34], [38].

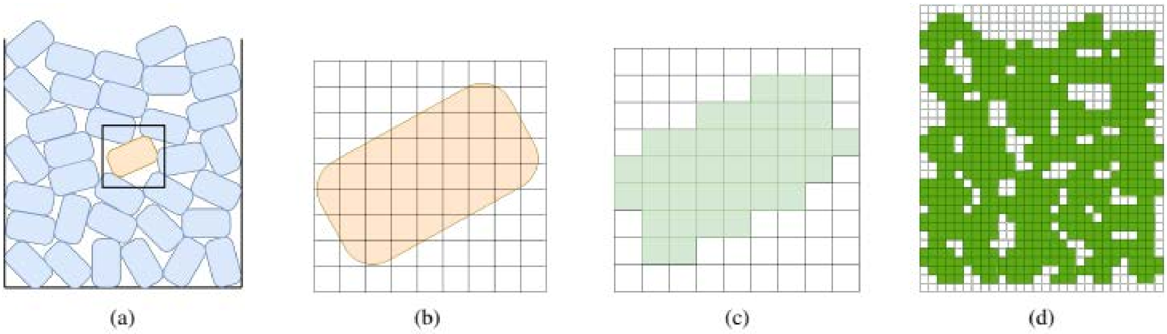


Figure 2.3: A simple representation of the steps involved in the voxelization of superquadric particles. (a) A single particle along with its bounding box is highlighted in the DEM data obtained from the simulation. (b) A zoomed in view of the highlighted particle, along with the bounding box containing the voxels. (c) Highlighting the voxels inside the particle. (d) Final voxel data after performing the preceding step for all the particles [39]**.**

A recent study by Pola [39] evaluated a voxelization-based post-processing methodology for analyzing the packing structure of non-spherical particle assemblies created from DEM simulations of superquadric or multisphere particles. In order to calculate the planar packing fraction, the authors first discretized the domain into a three-dimensional (3D) grid of small cubic elements called voxels (Figure 2.3). Then, they identified voxels found inside the particles. For this, the bounding box has been assigned for each particle. Once the voxels located at each point are determined, it is necessary to calculate the packing fraction. The packing fraction on the plane is the ratio of the number of voxels inside the particles to the total number of voxels on the plane.

In this work, a voxelization based post-processing methodology for DEM simulations was used to analyze the packing structure of the assembly.

2.6 Conclusion

Finally, the relevance of powder compact packing for engineering and materials science in creating and manufacturing excellent quality products cannot be overstated. The Discrete Element Method is well-known for being one of the most suitable methods for computing the structures of packing with irregular-shaped particles. Furthermore, it can address several features for the production of complicated particle forms in order to incorporate them into real cases. Superquadrics have been introduced as an effective approach for representing non-spherical shapes for generating their form.

As a result, the current study intends to provide a complete investigation of the effects of particle shape on the packing structure and the effect of amplitude and vibration frequency on the packing in order to realize process improvement. The enhanced voxelization approach for superquadric particles includes an algorithm for calculating the planar packing fraction along any arbitrary plane.

Chapter 3 – Methodology

3.1 Cylindrical particle generation

The cylindrical particles were created using the SQ technique. Particle shape and size are affected by superquadric geometric features such as half-lengths and sharpness indices. The superquadric parameters were set in order to generate cylindrical particles with similar volumes. The sizes of cylindrical particles, as well as the parameters used to generate them, are shown in Table 3.1.

Table 3.1: Dimension and parameters of cylindrical particles generated using SQ approach [27]**.**

Sample	Cylinder 1	Cylinder 2	Cylinder 3
			
d, mm	3	2.381	2.080
AR (h/d)	1	2	3
h, mm	3	4.752	6.240
V, mm^3	21.206	21.206	21.206
a, mm	1.5	1.191	1.04
b, mm	1.5	1.191	1.04
c, mm	1.5	2.381	3.12
n_1	10	10	10
n_2	2	2	2

3.2 DEM and simulation conditions

To model the packing of cylindrical particle mixtures, the Aspherix tool from DCS Computing GmbH [40] was used. Particle location and orientation are calculated using Newton's second law of motion. The translational and rotational motions of particles are explained by the following equations:

$$m_i \frac{d^2 x_i}{dt^2} = F_i \, , \tag{3.1}$$

$$L_i = T_i, \tag{3.2}$$

where m_i is the i^{th} particle mass, x_i is the particle position, t is time, F_i and T_i are the sums of forces and torques acting on the i^{th} particle, L_i is the angular momentum of the particle, $L_i = I_i \cdot \Omega_i, I_i$ is the tensor of inertia, and $\boldsymbol{\Omega_i}$ is the angular velocity in the observer-fixed coordinate system.

For irregularly shaped particles formulated as:

$$\hat{I}_i \dot{W}_i + W_i \cdot \hat{I}_i W_i = {A_i}^{-1} T_i, \tag{3.3}$$

where $\hat{I}_i$ is the particle tensor of inertia, W_i is the angular velocity, $W_i = {A_i}^{-1} \Omega_i$, and A_i is the rotation matrix defined in section 3.4 by equation (3.7).

The forces and torques affecting the particle are calculated as

$$F_i = F_{i,contact} + F_{i,gravity} + F_{i,external}, \tag{3.4}$$

$$T_i = T_{i,contact} + T_{i,external}. \tag{3.5}$$

The Hertz-Midlin contact model is used in the present study [13].

Table 3.2 provides the particle's mechanical and physical properties as well as the DEM simulation parameters. Binary mixtures of cylinder particles with different aspect ratios were simulated using 12,000 cylinders arranged in a container with the dimensions 0.064m × 0.064m × 0.13m (Table 3.3). A block region was created on the container's top, and cylindrical particles with random orientation were formed in the container to mimic the so-called poured packing conditions, in which packing is made by pouring particles into a vessel from the vessel top. The particles were then deposited into the container by gravity once the bottom block plane was removed. The simulation environment closely resembles the actual packing conditions.

Table 3.2: Mechanical properties of stainless-steel particles and parameters of DEM simulations [41]**.**

	Properties	Value
Container size	width × thick × height, [m]	0.064 × 0.064 × 0.13
Mechanical properties	Young`s modulus, [Pa]	2.2×10^8
	Poisson ratio	0.3
	Restitution coefficient	0.64
	Friction coefficient	0.6
DEM parameters	Time-step, Δt [s]	10^{-5}
	Gravity, g [m/s^2]	9.81
Particles physical properties	Density, [kg/cm^3]	7980

Table 3.3: Composition of binary mixtures of cylindrical particles

	Volume fraction of AR=1	**AR=1**	**AR=2**	**AR=3**
Binary mixture of AR=1 and AR=2	C=25%	3000	9000	0
	C=50%	6000	6000	0
	C=75%	9000	3000	0
Binary mixture of AR=1 and AR=3	C=25%	3000	0	9000
	C=50%	6000	0	6000
	C=75%	9000	0	3000

3.3 Vibration condition

This part of the simulation was focused on investigating the influence of vibration parameters on the binary mixtures. Table 3.4 demonstrates the DEM simulation settings. By arranging 6,000 cylinders in a container with a dimension of 0.064m × 0.064m × 0.26m, samples of binary mixtures of cylinder particles with varied aspect ratios (Table 3.5) were modeled. Mechanical and physical properties of cylindrical particles are the same as in the previous simulation.

Table 3.4: Vibration parameters of DEM simulations.

	Properties	Value
Container size	width × thick × height, [m]	0.064 × 0.064 × 0. 26
Vibration condition	Vibration frequency, ω [rad/s]	50-150
	Vibration amplitude, A [m]	0.004-0.012

Table 3.5: Binary mixtures composition for vibration

	Volume fraction of AR=1	AR=1	AR=3
Mixture 1	C=25%	1500	4500
Mixture 2	C=50%	3000	3000
Mixture 3	C=75%	4500	1500

The simulation started with poured packing of binary mixtures of cylindrical particles with random position and orientation in a rectangular box for 8 s under gravity for 800,000 time steps ($\Delta t=10^{-5}$) to achieve a compact packing. After packing a one-dimensional sinusoidal vibration governed by the equation:

$$\vec{x}(t) = \overrightarrow{x_0} + \vec{A}sin(\omega \Delta T), \tag{3.6}$$

where $\overrightarrow{x_0} = (x_0, y_0, z_0)$ is the mesh element position at the time when the vibration is activated, $\vec{A} = (A_x, A_y, A_z)$ is the amplitude vector, ω is the frequency, and ΔT is the time elapsed since the vibration was activated. Different vibration conditions can affect the dynamics of the vibration process. At this step, the vibration parameters (amplitude or frequency) are manipulated, which produced a number of simulations. The values of A and ω used in this work are 0.004-0.012 m and 50-150 rad/s. The vibration stops at 16 s, then the packing reaches a steady state by settling down for another 8 s.

3.4 Calculation of planar packing fraction

The packing density of a particle assembly on a certain plane is measured by the planar packing fraction. Particle data from DEM simulation, such as half length along the x, y, z coordinates, rotation matrix as quaternions and sharpness index as blockiness was used to derive planar packing fraction via voxelization approach.

The particle's orientation is specified using rotation matrix A, which translates coordinate vectors in global space to coordinate vectors in the body-fixed frame [29].

$$A = \begin{pmatrix} 1-2(q_2^2+q_3^2) & 2(q_1q_2-q_0q_3) & 2(q_1q_3+q_0q_2) \\ 2(q_1q_2+q_0q_3) & 1-2(q_1^2+q_3^2) & 2(q_2q_3-q_0q_1) \\ 2(q_1q_3-q_0q_2) & 2(q_2q_3+q_0q_1) & 1-2(q_1^2+q_2^2) \end{pmatrix}. \tag{3.7}$$

Here, q_0 , q_1 , q_2 and q_3 are the quaternions given as

$$q_0 = \cos\left(\frac{\alpha}{2}\right), q_1 = \hat{x}\cdot\sin\left(\frac{\alpha}{2}\right), q_2 = \hat{y}\cdot\sin\left(\frac{\alpha}{2}\right), q_3 = \hat{z}\cdot\sin\left(\frac{\alpha}{2}\right), \tag{3.8}$$

and $\widehat{(x,\ \hat{y},\ z)}$ is the unit vector defining the axis of rotation, and α is the rotation angle around this axis.

The Euler angles ϕ, θ and ψ can be calculated from quaternions as

$$\begin{bmatrix}\phi\\ \theta\\ \psi\end{bmatrix} = \begin{bmatrix} \tan^{-1}\left(\dfrac{2(q_0q_1+q_2q_3)}{1-2({q_1}^2+{q_2}^2)}\right) \\ \sin^{-1}\left(2(q_0q_2-q_3q_1)\right) \\ \tan^{-1}\left(\dfrac{2(q_0q_3+q_1q_2)}{1-2({q_2}^2+{q_3}^2)}\right) \end{bmatrix} \tag{3.9}$$

The domain was divided into voxels, and the voxels within the particles were identified. The packing fraction on the plane is defined as the ratio of the total number of voxels on the plane to the number of voxels contained within the particles.

3.5 Summary

To summarize, the simulations were carried out for the investigation of the morphology of vibrated and poured packed binary cylindrical particle mixtures using the new voxelization approach.

First, DEM simulations and the superquadrics approach were used to generate cylindrical particles with different aspect ratios and their mixtures with different volume fractions. The vibrational forces were applied in order to investigate the influence of the amplitude at the constant frequency and frequency at the constant amplitude on the packing density. A histogram of particle orientation comparison of poured packed and vibrated packed for each packing was built in order to see clearly how each particle orientation affects the packing density.

Second, the planar packing fraction distribution of mixtures was measured by the voxelization method. The research method gives results of local packing distribution along x, y and z directions for each packing.

Chapter 4 – Results & Discussion

The first part of the work is devoted to study the packing structure analysis of poured packed binary cylindrical particle mixtures. The influence of vibration amplitude and frequency on the packing of the binary mixture is discussed in the second part. The orientation of each cylindrical particle after applied vibrational forces are presented in the form of a histogram of the angle between the plane and the particle axes. The planar packing fraction analysis estimated the packing fraction on the plane along the x, y and z directions.

4.1 DEM Simulation and Results

Effects of aspect ratio and volume fraction. The packings of binary cylindrical mixtures with various volume percentages are illustrated in Figure 4.1. Figure 4.1 (b), (d) explains how the aspect ratio of the particles and the composition of the particle mixture affect the height of the packing. The mixture of cylindrical particles with close aspect ratios (AR=1 and AR=2) and the highest percentage of cylinders with AR=1 produced the densest packing of the lowest height. As a result, the packing density is reduced as a result of the elongated particles. The results of measuring the total voidage of packed samples using the voxelization approach are shown in Figure 4.2 as confirmation. When the volume percentage of elongated particles is reduced, the packing voidage generally decreases and the packings of the mixtures of cylinders with AR=1 and AR=2 are denser than those produced by mixtures of cylinders with AR=1 and AR=3.

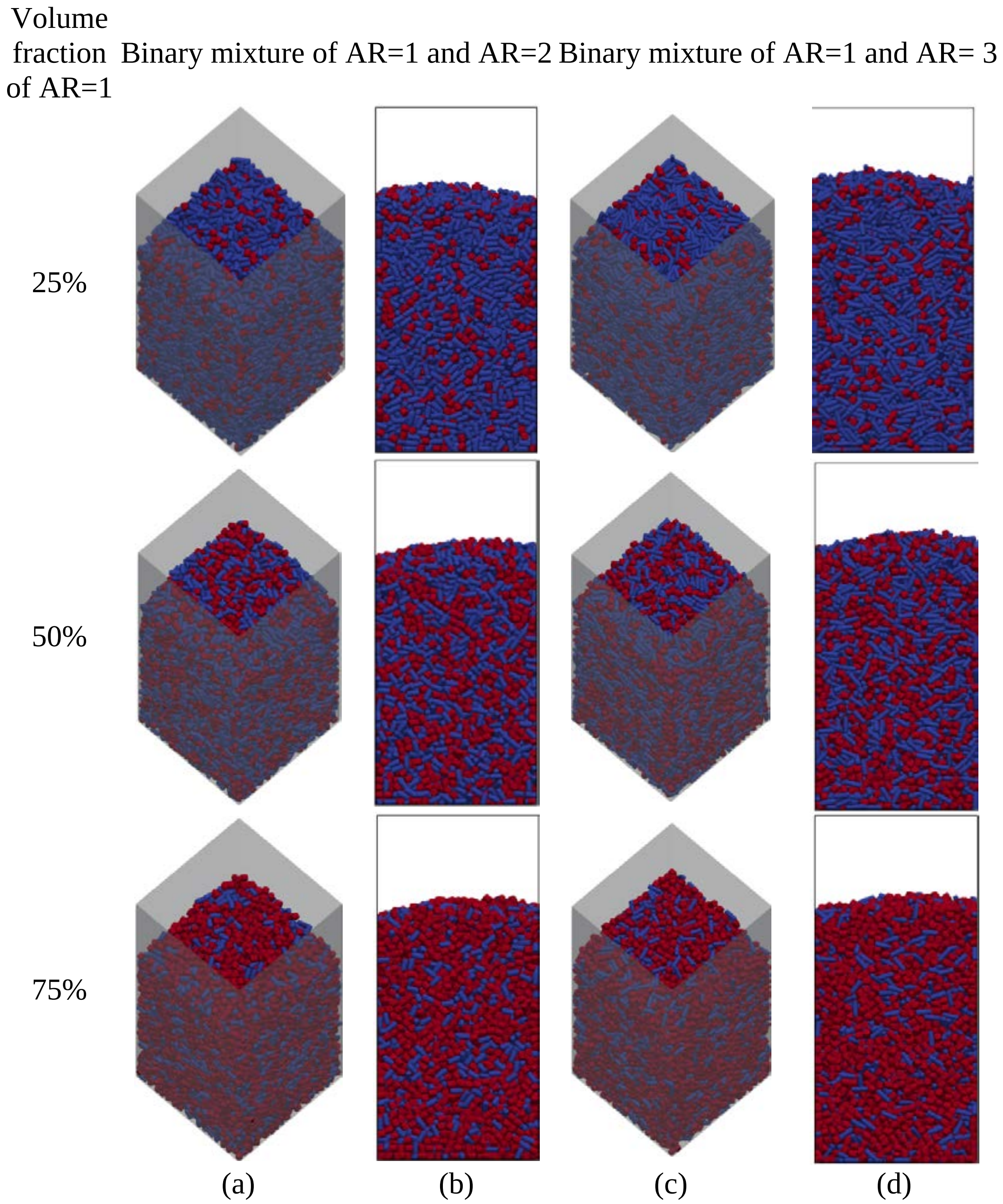


Figure 4.1: Visualization of binary mixtures of cylinders simulated using DEM: (a),(c) overall bed view and (b),(d) front view (red particles of AR=1, blue particles of AR=2 and AR=3).

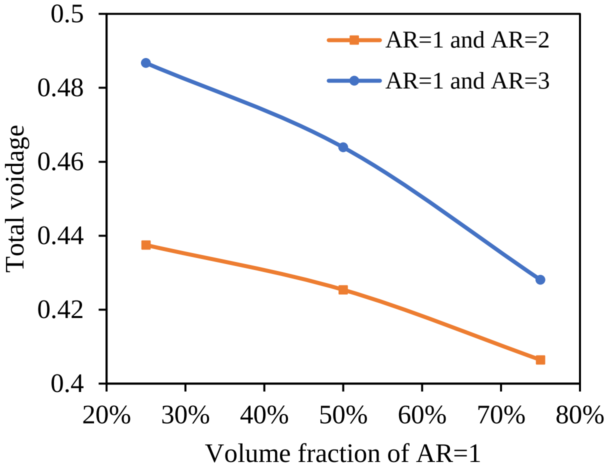
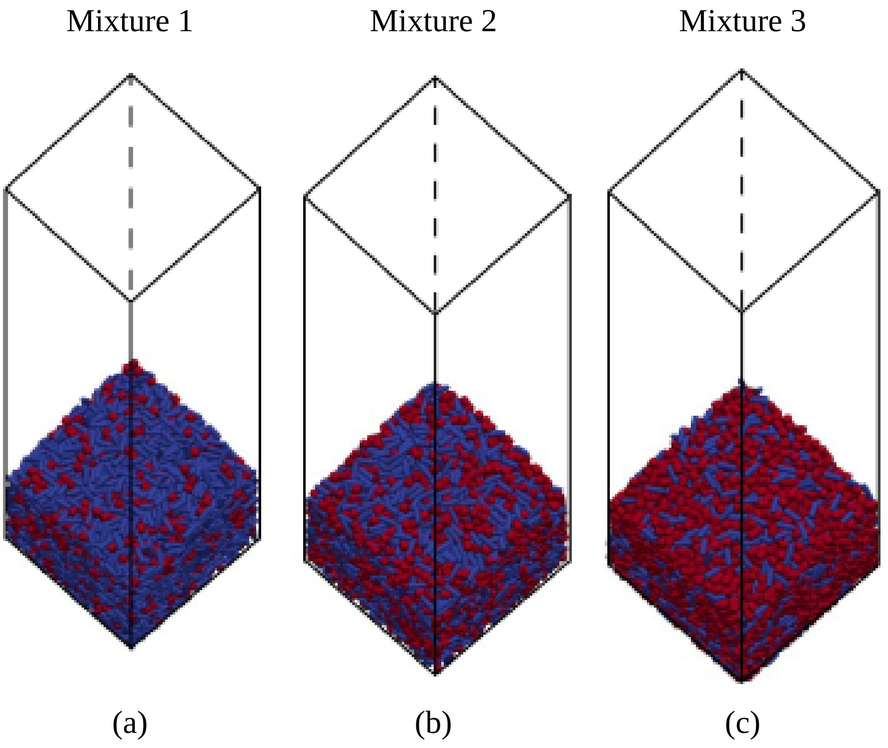
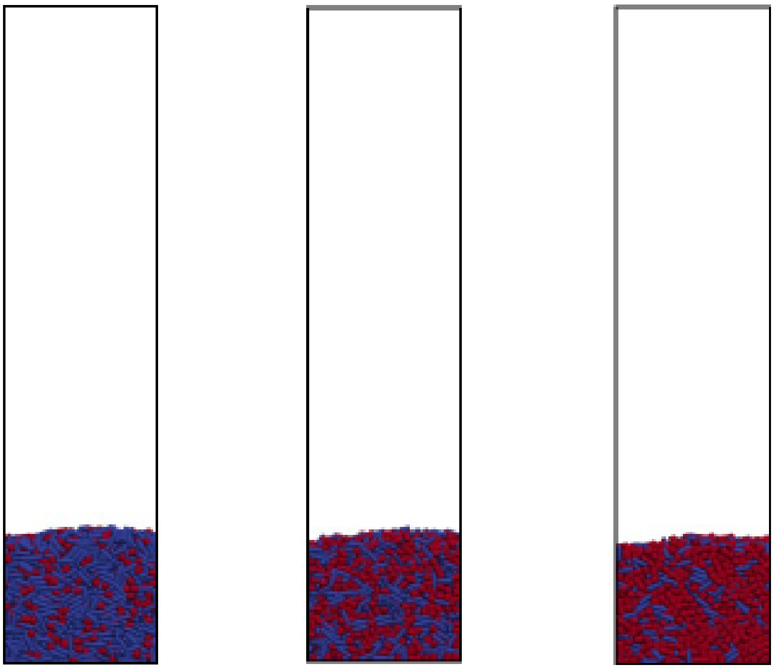


Figure 4.2: Total voidage of binary mixture of cylindrical particles

Effects of vibration conditions. Figure 4.3 shows the visualization of the randomly poured packings of binary cylindrical mixtures with different volume fractions. The total packing density of packed samples was measured by the voxelization method, and the results are demonstrated in Figures 4.4-4.5 for poured and vibrational packings of binary mixtures.





(d) (e) (f)

Figure 4.3: Visualization of binary mixtures of cylinders simulated using DEM: (a, b, c) overall bed view and (d, e, f) front view (red particles of AR = 1, blue particles of AR = 3).

The results show how varying the amplitude (Figure 4.4) at a constant frequency of 50 rad/s affects the packing density of three mixtures. The amplitude change is from 0.004 to 0.012 m. Densification for mixture 2 was obtained at packing density 0.555, at the amplitude value of 0.006 m. When the excitation is not high enough, particles do not move properly. When the oscillation is too large and the particles are distributed throughout the container, elongated particles create voids and particles with smaller AR can not fill voids. That is why at the amplitude range 0.004 – 0.012 m densification has not occurred in mixtures 1 and 3.

Similarly, a study was carried out to understand the effect of vibration frequency on the packing properties of binary mixtures. Amplitude was held constant at 0.006 m for mixtures, and frequency varied between 50-150 rad/s. The results for packing density are presented in Figure 4.5. For mixture 2 there is also densification obtained at 50 rad/s. Increasing vibration frequency led to overexcitation of particles and could not help to improve packing density. At 150 rad/s particles of mixture 1 jumped out of the container, therefore, the packing density for mixture 1 is not shown in the graph.

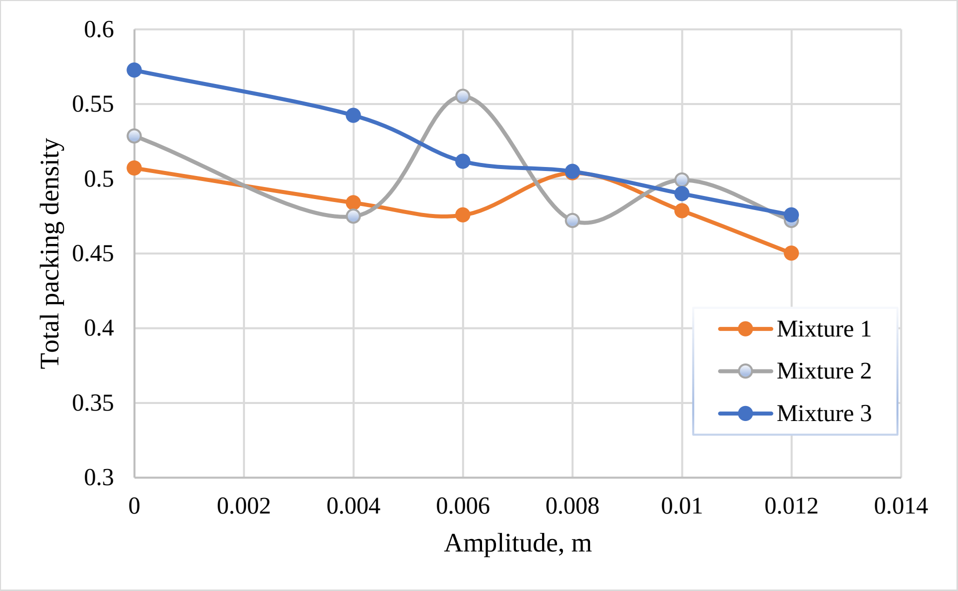


Figure 4.4: Total packing density of the binary mixture of cylindrical particles against amplitude at a constant frequency.

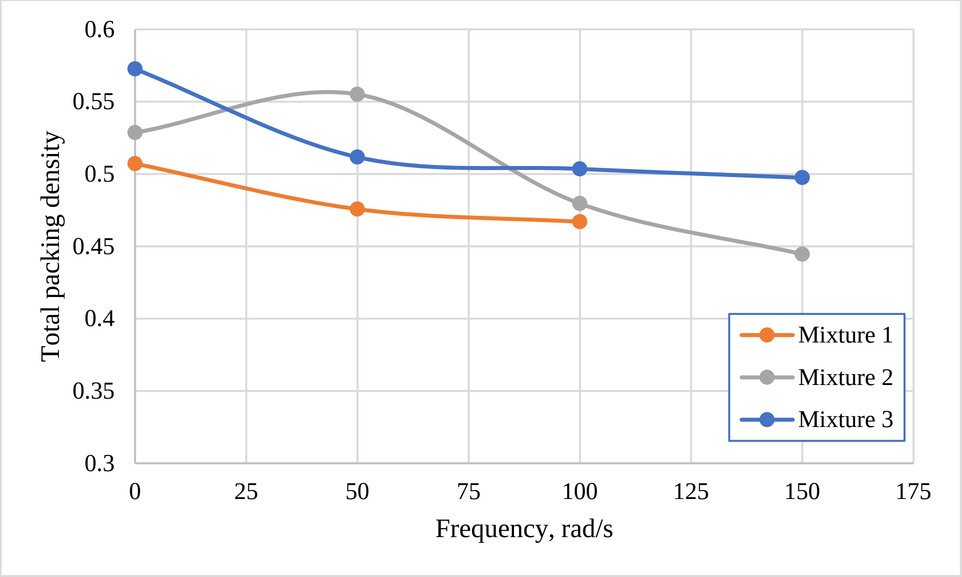
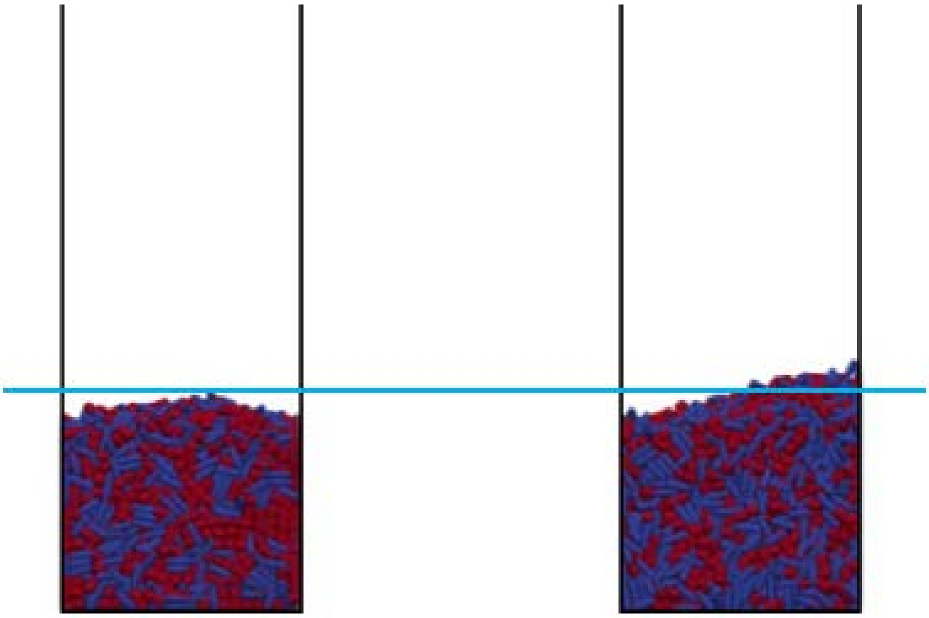


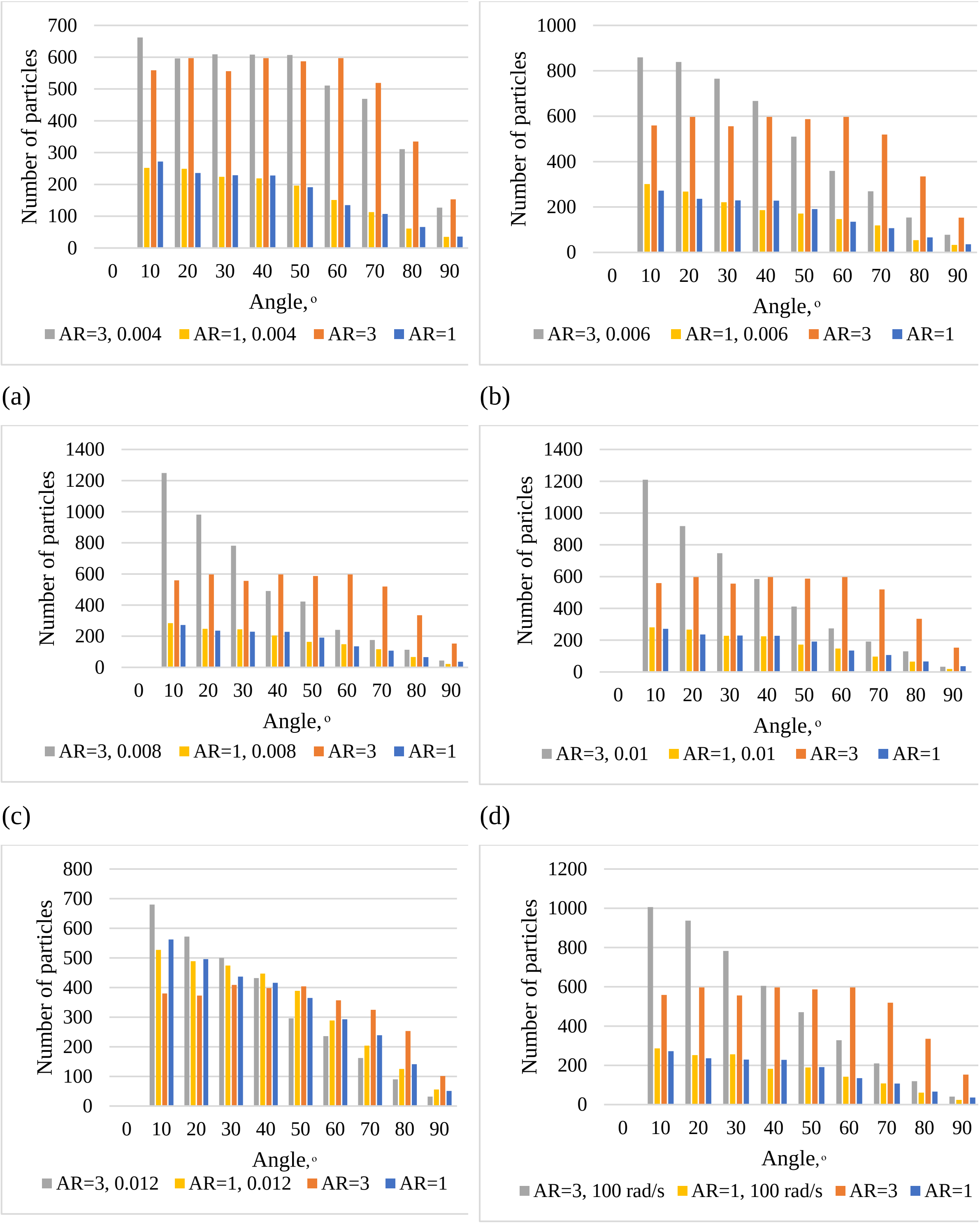
Figure 4.5: Total packing density of the binary mixture of cylindrical particles against frequency at a constant amplitude.



(a) (b)

Figure 4.6: Mixture 2 (a) A= 0.006 m, (b) A=0.012 m at ω = 50 rad/s.

The snapshots of mixture 2 at a different frequency and constant amplitude are shown in Figure 4.6. The line shows the level of packing at 0.006 m amplitude. It can be seen how the higher vibration amplitude can change the orientation of particles and shift the peak to the left, which can lead to a decrease in the packing density. To confirm that, the orientation of cylindrical particles at poured packing compared to vibrational packing is demonstrated in figures 4.7-4.9 in the form of a histogram of the angle between the horizontal plane and the particle axes. Here, an angle of 0◦ corresponds to the vertically oriented particle and an angle of 90◦ to the horizontally oriented one. Initially, during the formation of packing by pouring, the particles are randomly oriented. From orientations of poured packed particles, it can be seen that particles with a low aspect ratio, AR=1, are mainly oriented vertically, and with a high aspect ratio, AR=3, are more randomly oriented horizontally. After applying vibration, we can observe that particles change their position and tend to orientate vertically, which is prove for created voids and lowered packing density. Figure 4.7 shows the particle orientation for mixture 1, where the volume fraction of particle AR=3 was 75%. At the vibration amplitude range 0.006 - 0.010 m (Figure 4.7 (b-d, f)) it can be noticed how significantly move elongated particles in their position compared to poured packing. Similarly, from figure 4.9 it is clearly seen how particles with a small aspect ratio change their position under the vibrational forces.

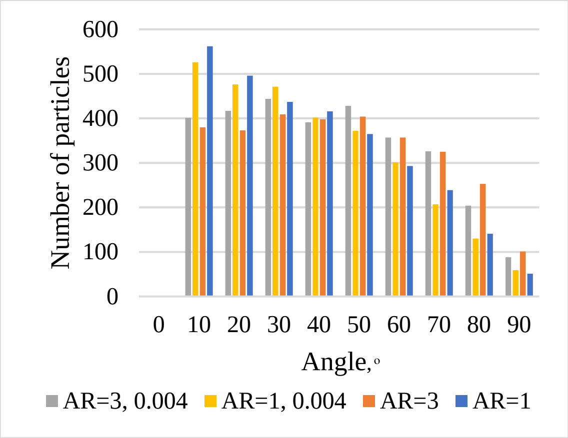


(a) (b)

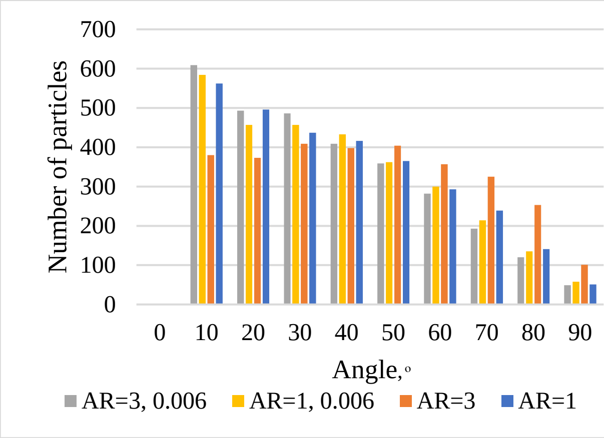
(c) (d)

(e) (f)

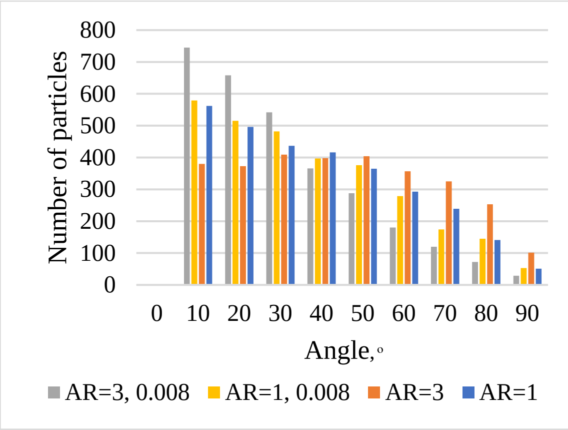
Figure 4.7: Histogram of particle orientation comparison of poured packed and vibrated packed Mixture 1: (a)-(e) different amplitude and constant frequency of ω =50 rad/s, (f) 100 rad/s frequency and amplitude of A=0.006 m.


Number of particles
600
500
400
300
200
100
0
0 10 20 30 40 50 60 70 80 90
Angle,°
■ AR=3, 0.004 ■ AR=1, 0.004 ■ AR=3 ■ AR=1

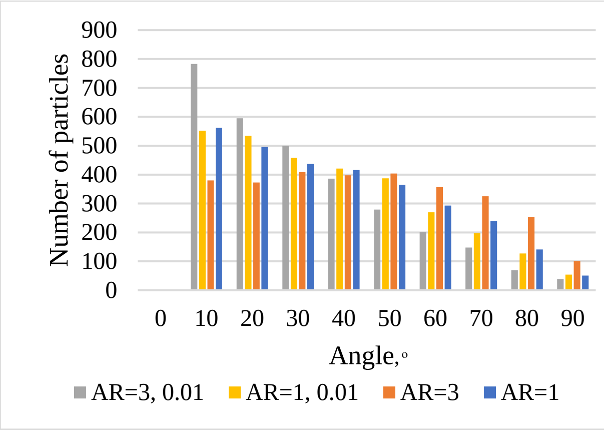
(a)


Number of particles
700
600
500
400
300
200
100
0
0 10 20 30 40 50 60 70 80 90
Angle,°
■ AR=3, 0.006 ■ AR=1, 0.006 ■ AR=3 ■ AR=1

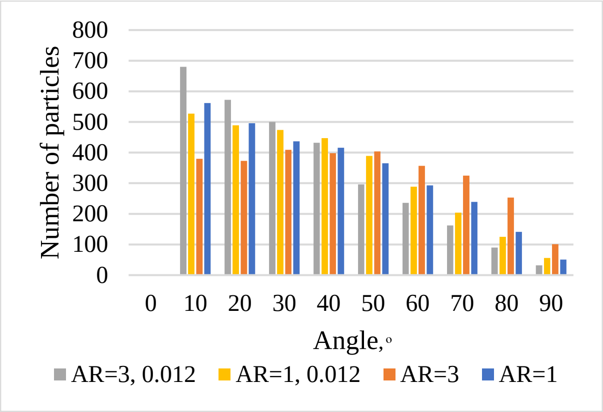
(b)


Number of particles
800
700
600
500
400
300
200
100
0
0 10 20 30 40 50 60 70 80 90
Angle,°
■ AR=3, 0.008 ■ AR=1, 0.008 ■ AR=3 ■ AR=1

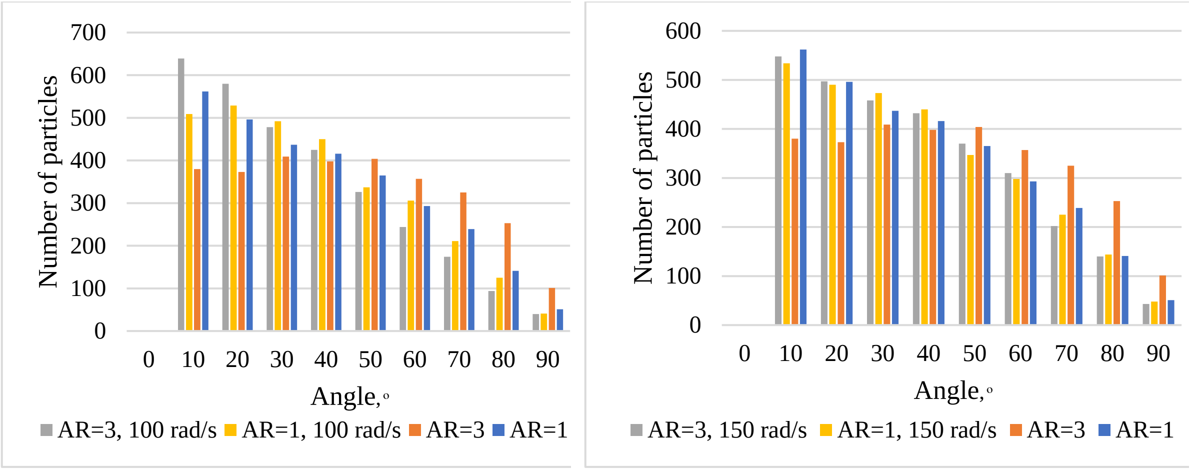
(c)


Number of particles
900
800
700
600
500
400
300
200
100
0
0 10 20 30 40 50 60 70 80 90
Angle,°
■ AR=3, 0.01 ■ AR=1, 0.01 ■ AR=3 ■ AR=1

(d)

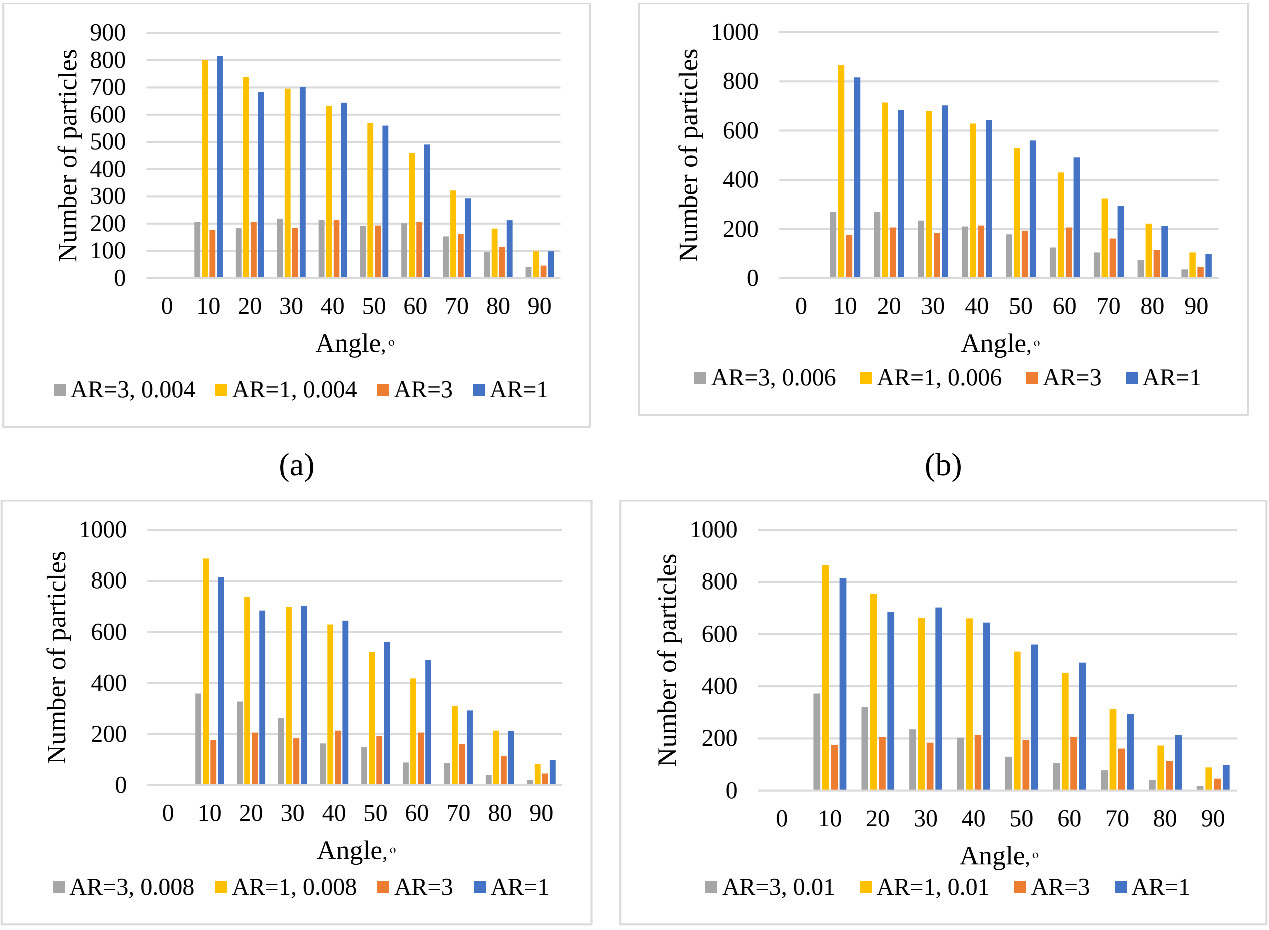

Number of particles
800
700
600
500
400
300
200
100
0
0 10 20 30 40 50 60 70 80 90
Angle,°
■ AR=3, 0.012 ■ AR=1, 0.012 ■ AR=3 ■ AR=1

(e)



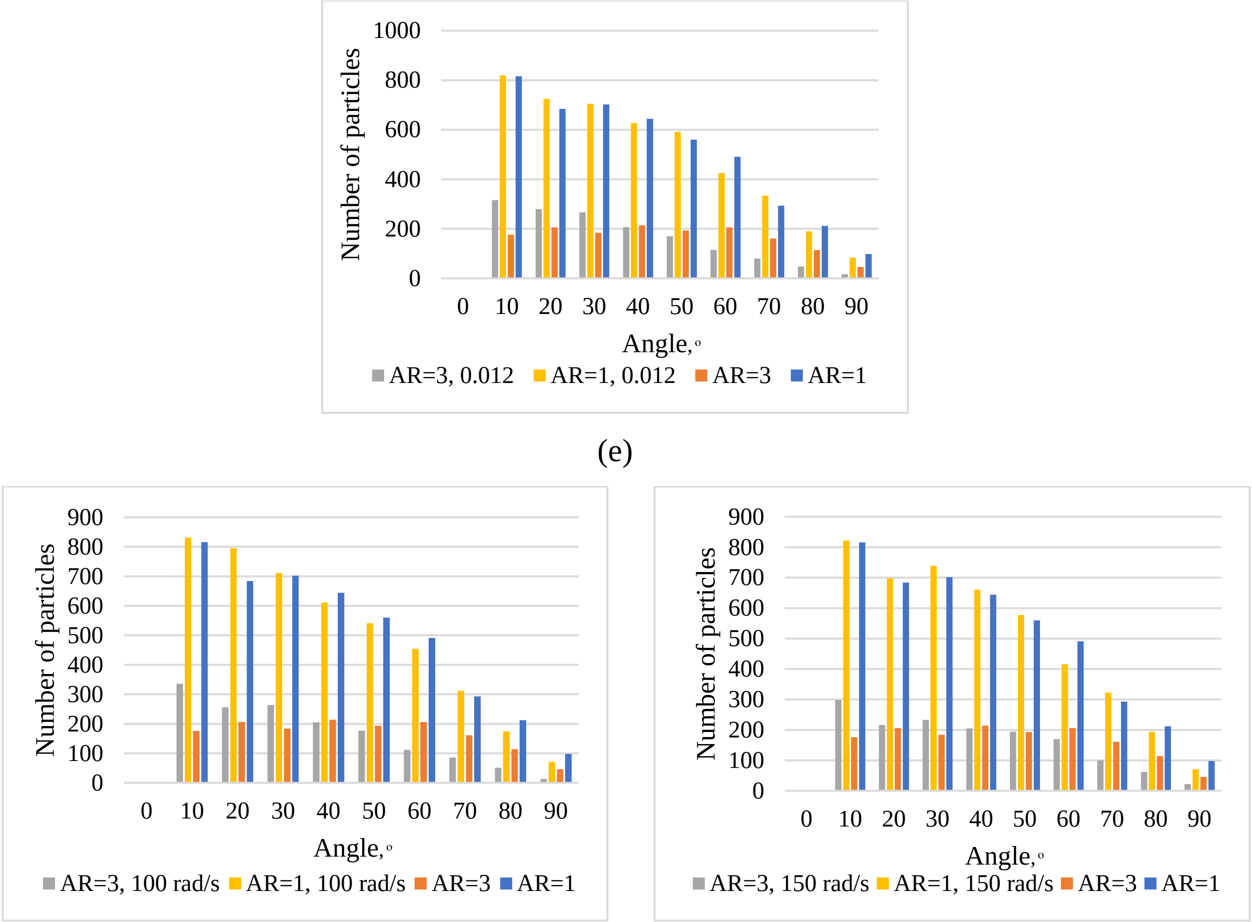
(f) (g)

Figure 4.8: Histogram of particle orientation comparison of poured packed and vibrated packed Mixture 2: (a)-(e) different amplitude and constant frequency ω =50 rad/s, (f)-(g) different frequency and constant amplitude A=0.006 m.



(a) (b)

(c) (d)



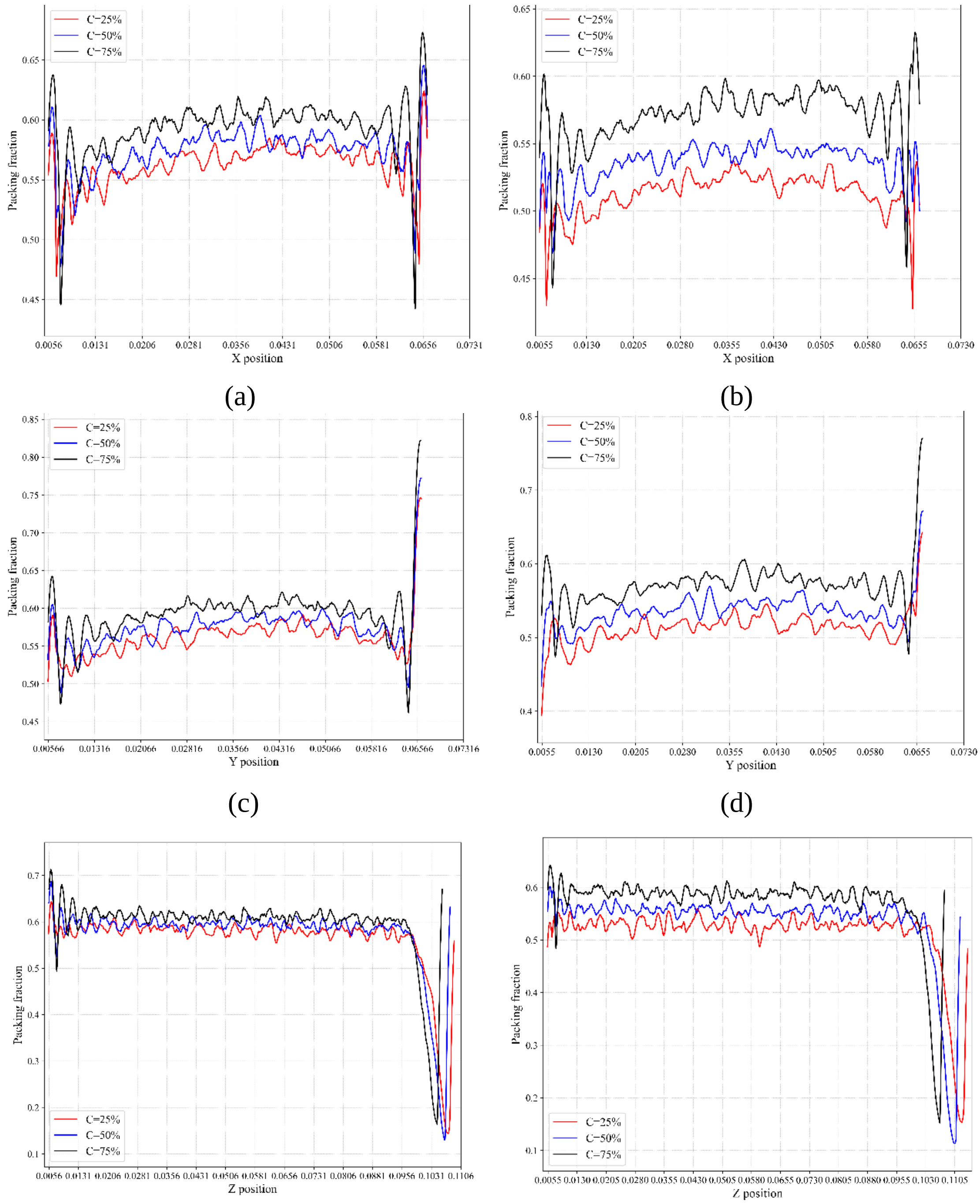
(e)

(f) (g)

Figure 4.9: Histogram of particle orientation comparison of poured packed and vibrated packed Mixture 3: (a)-(e) different amplitude and constant frequency of ω=50 rad/s, (f)-(g) different frequency and constant amplitude of A=0.006 m.

4.2 Planar Packing Fraction

Effects of aspect ratio and volume fraction. The investigation of the packing fraction variation plots for packings of cylindrical particles reveals a weak wall effect (Figure 4.10). For packings in the x and y directions, two noticeable peaks may be observed adjacent to the side walls, suggesting poor mating of the curved particle surfaces against the flat wall surface. The fact that the packing percentage in the z direction rapidly drops off at the end, shows that the particles at the top of the container are not packed uniformly. Comparing patterns of planar packing fraction distributions for mixtures of various compositions can show how the aspect ratio of cylindrical particles affects packing microstructure. The higher the aspect ratio of the cylinders constituting the binary mixture, the less the packing fraction distribution of mixtures of various compositions differs from one another.



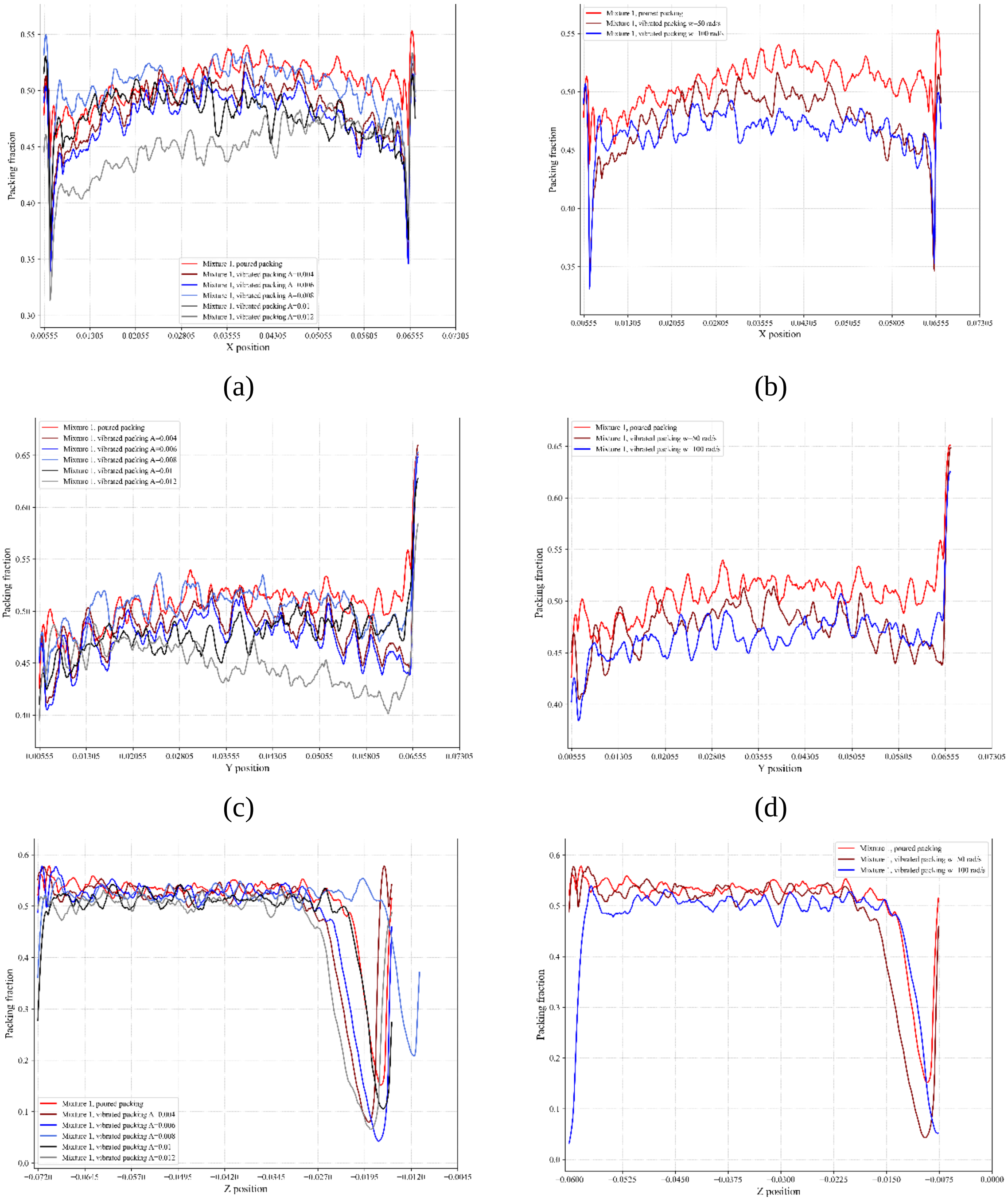
(a) (b)

(c) (d)

(e) (f)

Figure 4.10: Packing fraction along x,y,z direction for (a), (c), (e) binary mixtures of AR=1 and AR=2, and (b), (d), (f) binary mixtures of AR=1 and AR=3.

Effect of vibration conditions. Figures 4.11-4.13 demonstrate the change of packing fraction along x, y and z directions at different vibration conditions. Results in the packing fraction along the x, y direction for mixtures demonstrate with increasing vibration amplitude or frequency, particles are not distributed evenly throughout the domain and top particles tend to move to one side of the wall. From packing fraction along the z direction, vibration amplitude or frequency does not significantly change the packing density of bottom particles. Top particles are over-excited, and their movement led to producing loose packing.

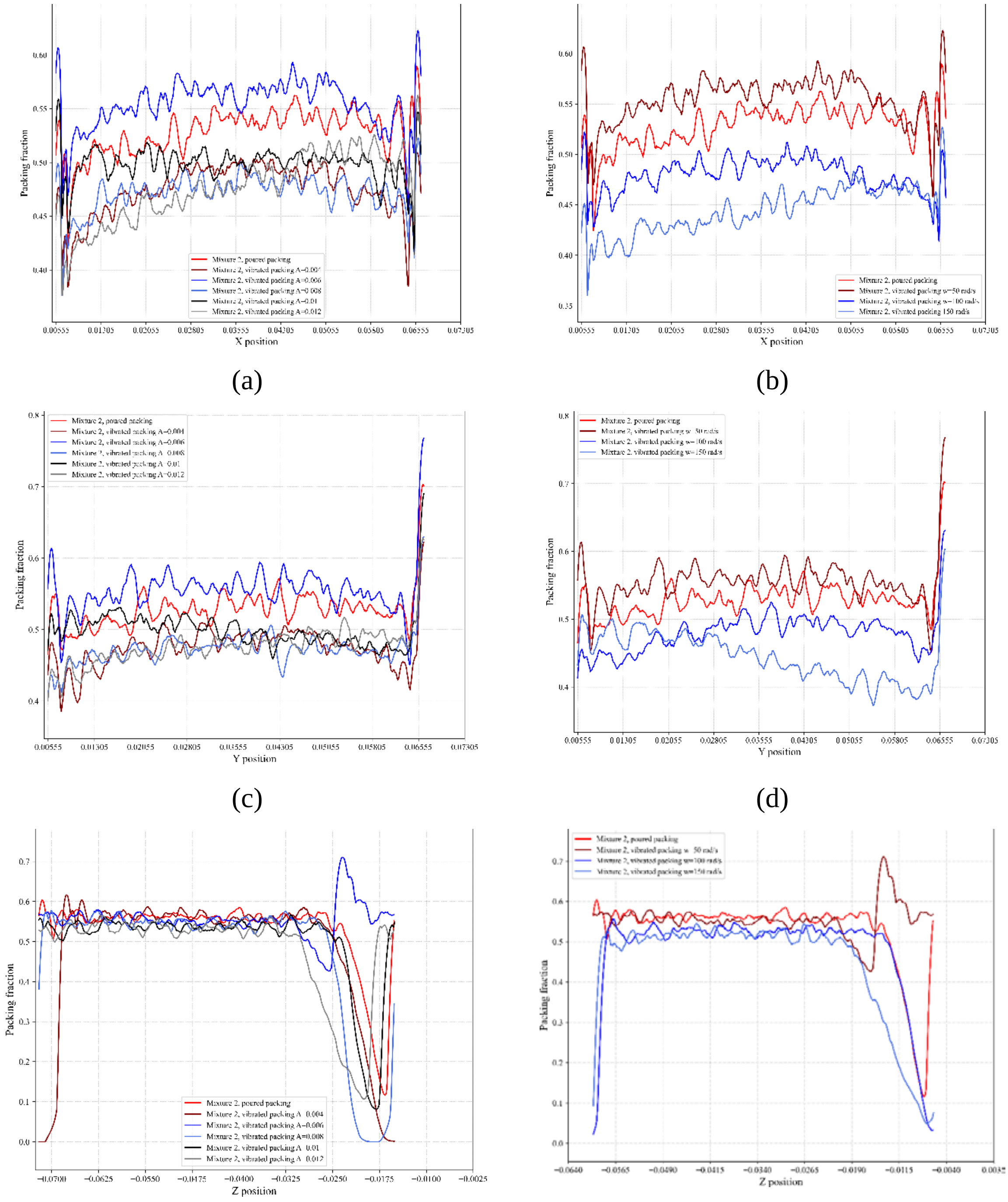


(a) (b)

(c) (d)

(e) (f)

Figure 4.11: Packing fraction along x,y,z direction for mixture 1 (a), (c), (e) different amplitude and constant frequency of ω=50rad/s, (b), (d), (f) different frequency and constant amplitude of A=0.006 m.

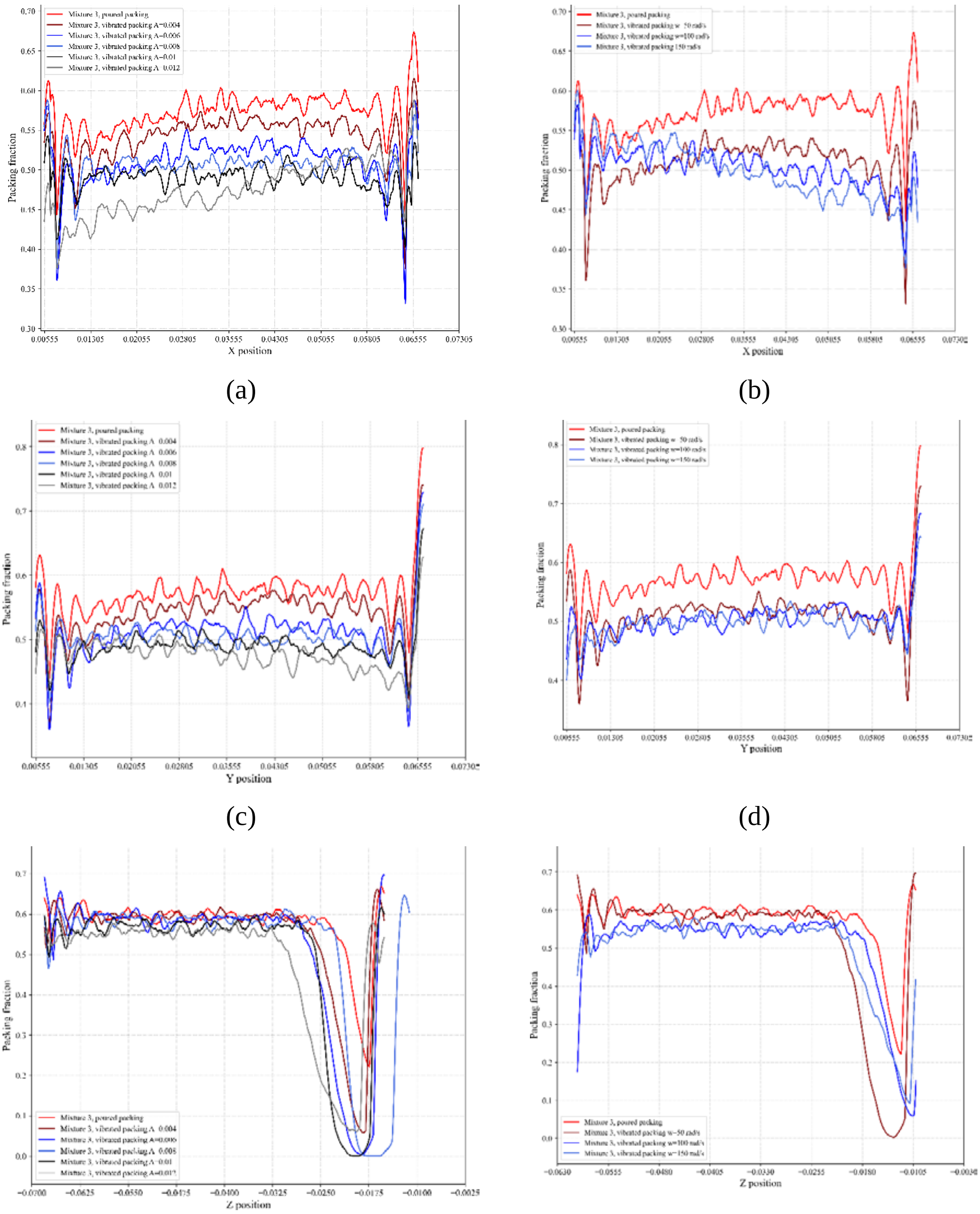


(a) (b)

(c) (d)

(e) (f)

Figure 4.12: Packing fraction along x,y,z direction for mixture 2 (a), (c), (e) different amplitude and constant frequency of ω=50rad/s, (b), (d), (f) different frequency and constant amplitude of A=0.006 m



(a) (b)

(c) (d)

(e) (f)

Figure 4.13: Packing fraction along x,y,z direction for mixture 3 (a), (c), (e) different amplitude and constant frequency of ω=50rad/s, (b), (d), (f) different frequency and constant amplitude of A=0.006 m

4.3 Summary

To sum up, the effects of the volume fraction and aspect ratio of particles on the packing structure were measured and the influence of the vibration conditions, such as amplitude and frequency, on packing density were analyzed. The orientations of cylindrical particles in the poured packing compared to vibrational packing were demonstrated in the form of a histogram of the angle between the horizontal plane and the particle axes, while the packing microstructure was analyzed through the voxelization approach. The total packing density was also calculated.

Packings of binary mixtures of cylindrical particles were generated under gravity. In the first part of the work, binary mixtures of cylindrical particles were generated and the impact of the volume fraction and aspect ratio on the packing density was studied. The next step was to evaluate the impact of vibration amplitude and frequency on the packing characteristics of each mixture. The amplitude range varied between 0.004-0.012m at a constant frequency of 50 rad/s, and the frequency was between 50-150 rad/s at a constant amplitude of 0.006 m.

Study on the aspect ratio and volume fraction of cylindrical particles in the mixture

The results demonstrate that mixtures with particles with a higher aspect ratio and mixtures with a higher percentage of elongated cylindrical particles produce less dense packings. The planar packing fraction curves show that 75% of elongated particles mixed with the 25% cylinders with AR=1 demonstrate the lowest packing fraction.

Study on the vibration effect on packing density

The total packing density of three mixtures was calculated for each vibrational condition. The densification for mixture 2 was achieved at conditions A=0.006 m, ω= 50 rad/s. Particles of mixture 2 over-exited as amplitude and frequency increased, resulting in a loose packing structure. For mixtures 1 and 3, it was not possible to achieve densification at the given vibration conditions. This is explained by the change in particle orientation. To confirm that, a histogram of the angle between the horizontal plane and the particle axes was performed. It was found that after applying vibrational forces particles change their position and tend to orientate vertically, which creates voids and lower packing density.

To study the impact of vibration conditions on binary mixtures in more detail, the packing fraction of mixtures were analyzed by the voxelization method. Packing fraction along x and y directions demonstrated the displacement of particles near to one side of the wall at high vibration amplitude or frequency, which lead to an increase in the bed height and a decrease of the packing density. The vibration amplitude and frequency do not much change the packing fraction of bottom particles, while top particles over-excite, which forms loose packing.

Finally, the binary mixtures of cylindrical particles with different aspect ratios and volume fractions were studied at various vibration conditions. The simulation results show that the fraction of elongated particles in a binary mixture can influence the packing structure and the vibration amplitude and frequency can influence the packing density of binary cylindrical particle mixtures by changing the orientation of cylindrical particles in the packing.

Chapter 5 – Conclusions and Recommendations

To sum up, the thesis work consists of the literature review, methodology, results and discussion parts which dedicate to analyzing the effects of vibration parameters on the binary mixtures of cylindrical particles. The literature review discusses various methods used to generate packings of cylindrical particle mixtures. Thus, from the literature review the DEM was used as the modeling approach for the simulation of packings. The influence of vibration amplitude and frequency was explained by the orientation of the particles and packing fraction analysis. The simulation parameters were controlled according to cost and time efficiency concerns with the chosen approaches.

The first part of the research work covered the simulation part of binary mixtures of cylindrical particles with different aspect ratios and volume fractions under gravity. The second part was dedicated to the simulation of vibrated packing of mixtures at varying amplitude, constant frequency and different frequency, constant amplitude.

The study applies DEM simulation for the generation of cylindrical particles with the same volume but different aspect ratios and packings of three binary mixtures consisting of 12000 cylindrical particles with varying volume fractions. Packing microstructure was systematically analyzed by voxelization. The findings show that mixtures with more elongated cylindrical particles and mixtures of particles with higher aspect ratios generate less dense packings. The planar packing fraction curves reveal that the lowest packing fraction is produced by a mixture of 75% elongated particles and 25% cylinders with AR=1.

Then, the vibrational forces were utilized for further analysis of densification characteristics. The amplitude range varied between 0.004-0.012m at a constant frequency of 50 rad/s, and the frequency was between 50-150 rad/s at a constant amplitude of 0.006 m. For each vibrational state, the total packing density of three mixtures was determined. The densification for mixture 2 was determined at $A=0.006$ m, $\omega=50$ rad/s. At increasing amplitude and frequency, particles of mixture 2 over-excited, resulting in a loose packing structure. Packing density of mixtures 1 and 3 decreased after vibration. This is explained by the change of orientation of cylindrical particles. To prove that, a histogram of the angle between the horizontal plane and the particle axes was created. It was discovered that vibration parameters can impact the orientation of cylindrical particles, they tend to orient vertically, resulting in created voids and decreased packing density.

To investigate the influence of vibration conditions on the morphology of powder compacts binary mixtures of cylindrical particles in more depth, the packing fraction of mixtures was examined using the voxelization approach. Analysis of packing fraction distribution along the x and y axes revealed a displacement of the particles to one side of the wall at high vibration amplitude or frequency, which caused an increase in bed height and a decrease in packing density. The vibration amplitude and frequency have almost no effect on the packing fraction of bottom particles, whereas top particles over-excite, resulting in loose packing.

Future Recommendations

Further research needs to be provided for the evaluation of densification with a wider range of vibration amplitude and frequency. Furthermore, mixtures with different aspect ratios and sharpness of superquadric shapes can also be implemented in order to analyze the influence of shape parameters on the packing density. The container geometry can be changed in order to examine the impact of container size and the wall on densification. In addition, despite still limited numbers of algorithms based on Voronoi tessellation, it can be applied to determine packing microstructure on binary cylindrical mixtures in detail.

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