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Packing Structure of Binary Particle Compacts with Fibers

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Abstract. Fibers have been used to improve the mechanical properties of the asphalt paving mixture. It is known that the enhancement of powder compact mechanical properties is related to the compact packing microstructure. This study focuses on the evaluation of the packing microstructure of powder compacts produced from ternary mixtures of spherical particles and fibers. The discrete element method is employed to generate the compacts of particle mixtures of different compositions under gravity. The compact microstructure is quantitatively characterized by utilizing the developed image analysis technique to approximate the size distribution of voids among particles in X, Y and Z directions. As a result, the denser packing was obtained with a greater fraction of small spherical particles. The inclusion of fibers resulted in the high-density compact with uniform distribution of small size voids.

1. Introduction

Asphalt paving mixture has been in wide use for the production of materials with a strong adhesion effect. The asphalt mixture mainly consists of various sized aggregates. In spite of mechanically strong properties, asphalt pavement is generally affected by a significant traffic load stress leading to irreversible damages and cracking of the surface [1, 2]. Due to the flexibility decrease causing strong deformations [3, 4], the reinforcing of mechanical characteristics of asphalt mixture has become a topical question.

The incorporation of fibers can enhance the consistency of asphalt paving mixture and, thus, significantly improve the mechanical properties of the mixture [5]. Fiber additives have shown good resistance to leakage and drainage through improving the stability of entire mixtures [5, 6]. Moreover, the fibers can be used to lessen various problems with mechanical properties such as dynamic and static stabilities, ductility, and general physical characteristics [7]. It is also known that the aggregate size distribution can have a significant effect on improving the engineering properties of a material [8]. There is still a need in quantitative analysis of the microstructure of powder compact consisting of differently sized particles and fibers, and in research that eventually relates the microstructural parameters to the compact mechanical properties.

Recently, numerical methods have been successfully applied to the investigation of the asphalt compact microstructure due to their cost effectiveness, controlling patterns, and large amounts of data generated. One of the methods to simulate particle packing is a Discrete Element Method (DEM). In early papers, the simulations were conducted with monodisperse spherical particles and only simple interactions between them were taking into account. Lately, DEM has been improved to model more realistic particulates with various characteristics [9, 10]. Yi et al. [9] and Zhu et al. [10] pointed out that it allows accumulating better representation of the dynamical process during compaction in



comparison with experimental techniques. The DEM has been recently used to simulate the packing and flow of hot mix asphalt mixtures [11-13].

The objective of this study is to investigate the microstructure of powder compact produced from the ternary mixture of spherical and fiber particles. The DEM will be used to generate the packing structure and the superquadrics approach will be utilized for the creation of spherical and elongated ellipsoidal particles. The compact microstructure will be characterized quantitatively using the size distribution of voids among particles. The image analysis procedure and software will be developed to measure the void size distribution on compact cross-sections in X, Y, and Z directions.

2. Methodology

2.1. Particle generation

In our simulations, the powder compacts consist of the fine and coarse spherical particles with 4 mm and 8 mm in diameters, respectively, and elongated fibers with 12 mm in length. The densities of spherical and fiber particles are 2.257 g/cm³ [14] and 1.140 g/cm³ [15], respectively.

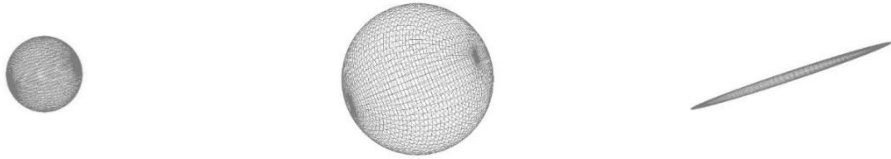
The elongated ellipse-shaped particles are used to represent the fibers. The spherical and ellipsoidal particles were created by using a superquadrics approach [16]:

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

where a , b and c corresponds to the half-length of the particles, i.e., the radii of fine and coarse particles, and the length of the semi-major ellipse axis, respectively, n_1 and n_2 reflects the sharpness of the particles, and $f(x, y, z)$ is the shape function defined in the local coordinate system. Table 1 illustrates the particle shapes created by the superquadrics builder tool in CFDEM®WORKBENCH software [17, 18].

There are several techniques to increase the time-efficiency of computation, such as controlling the particle shape parameters, size of the particles, managing the overlap between particles, etc. Our preliminary simulations confirmed that the addition of small fibers to the powder mixture results in a significant increase in simulation time owing to the necessity to use a very small time step in DEM simulations. As a consequence, the size of fiber particles has been enlarged to achieve reasonable simulation time.

Table 1. Visualization of spherical and fiber particles created using superquadrics.

Particles			
			
	Fine spherical	Coarse spherical	Fibers
	Superquadrics parameters		
a , m	0.002	0.004	0.0002875
b , m	0.002	0.004	0.0002875
c , m	0.002	0.004	0.006
n_1	2	2	2
n_2	2	2	2

2.2. DEM simulation setup

The mechanical properties of particles and DEM simulation parameters were taken from Soltanbeigi et al. [16] (see table 2). To study the effect of fibers inclusion on packing structure, DEM simulations

have been carried out using the GUI CFDEM®WORKBENCH interface to LIGGGHTS [18] software for four specimens with different mixture composition, as summarized in table 3.

Table 2. The mechanical properties of particles and DEM simulation parameters.

Mechanical properties	
Young's modulus, [Pa]	10^7
Poisson ratio	0.3
Restitution coefficient	0.6
Friction coefficient	0.3
DEM parameters	
Time-step, Δt [s]	4×10^{-6}
Gravity, g [m/s ²]	9.81

Table 3. Particle mixture composition for DEM simulations.

Run	Fiber, wt. %	Fine, wt. %	Coarse, wt. %
1	0	63	37
2	1	62	37
3	0	40	60
4	1	40	59

2.3. Analysis of packing structure of powder compact

The packing structure of the ternary mixture of small and large spherical particles and fibers was estimated quantitatively using the concept of void size distribution [19]. The void size distribution is related directly to the packing structure of powder compact [20-22]. The following algorithm was developed to evaluate the size distribution of voids among particles. At first, the three-dimensional image of powder compact simulated using DEM software was visualized in the open-source Paraview software [23]. Then, the Slice Cut function of Paraview was employed to extract the cross-sections of ternary mixture compact taken along with the three axes X, Y, and Z in normal positions. Then, the open-source image analysis software ImageJ [24] was used to convert the color images of cross-sections into the binary images required for subsequent processing. The color images were processed by smoothing images and reducing noise for the clear separation of particles from the void phase. Finally, the distribution of void sizes in a two-dimensional cross-section was measured by randomly placing the void circles of various sizes all over the binary image. The trial was count as a successful one if the circle does not overlap the particle or touch the particle boundary. Then, the probability of the existence of the void of particular size was defined as the ratio of successful trials to the total number of trials. The total number of trials for each circle size was selected as 30,000 based on our preliminary study. The macro program for ImageJ was developed to measure the void size distribution. The examples of cross-section images of powder compact before and after binarization are shown in figure 1. The cross-sections of the compact of a binary mixture of spherical particles are illustrated in figures 1 (a) and 1(b) and the cross-sections of the compact of a ternary mixture of spherical particles and fibers are shown in figures. 1(c) and 1(d). The fibers are clearly seen in figure 1(d), and the particle and fibers outlines in figure 1 (d) are similar to those in figure 1(c) confirming the successful image preparation and binarization procedure.

The microstructure of powder compact was analysed using the cross-sections taken at the same position in the compact in three planes perpendicular to X, Y and Z axes. The area based void size distributions were measured on each cross-section and the distribution parameters were evaluated including the median void size, d_{50} , corresponding to 50% value on the cumulative frequency distribution curve and the distribution sharpness index defined as a ratio d_{90}/d_{10} , where d_{10} and d_{90} are the void diameters corresponding to 10% and 90% of cumulative frequencies, respectively.

3. Results and discussion

3.1. DEM simulation results

Figure 2 illustrates the powder compact generated by DEM simulation and visualized by Paraview for the mixtures of spherical particles (figure 2(a)) and spherical particles and fibers (figure 2(b)) with various fractions of fine and coarse components. The fibers are distributed throughout the compact and the fibers are mainly oriented along with the X and Y directions, as confirmed in figure 2(b).

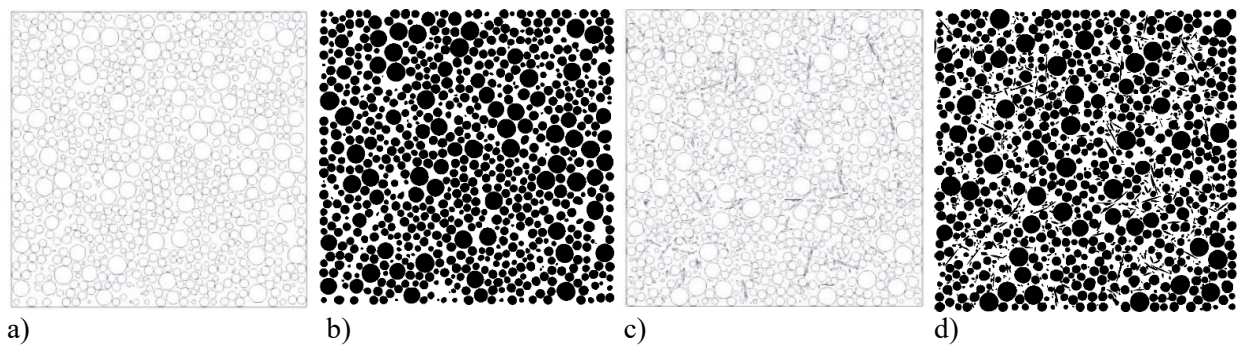


Figure 1. Images of cross-sections normal to Z direction: (a) compact cut from DEM and (b) binary image for Simulation 1, and (c) compact cut from DEM and (d) binary image for Simulation 2.

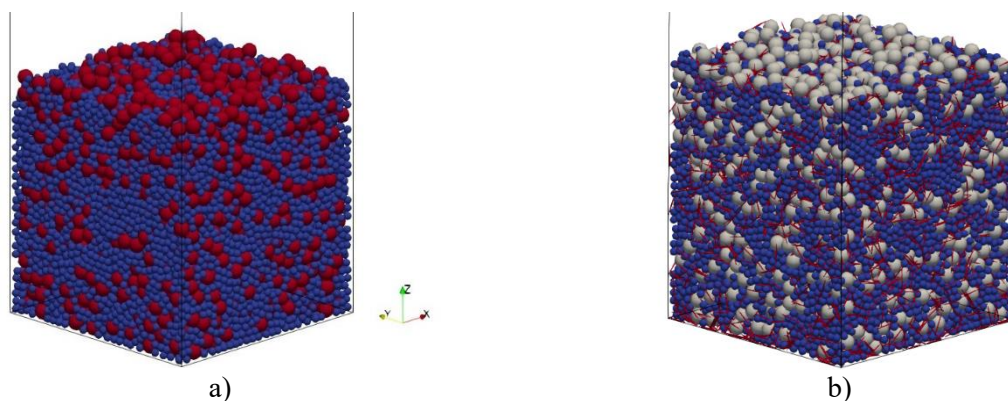


Figure 2. The images of packing structure for (a) Simulation 2 and (b) Simulation 4 in Paraview.

3.2. The microstructure of powder compacts

3.2.1. Binary mixtures of spherical particles. The cumulative frequency void-size distributions measured in X and Y directions on compacts of binary mixtures of spherical particles are shown in figure 3. The median sizes and sharpness indices are summarized in table 4. The ratio of fine and coarse particle sizes was kept constant as 1:2, but the weight fraction of fine particles was varied from 63% (Simulation 1) to 40% (Simulation 3).

The similar trends are observed for packing structures of powder compacts in all directions. The packing densities increases, the size of voids among particles decreases and the voids are more uniformly distributed in the packings of particle mixture with a large amount of fine particles. The median void size decreases from 1.068 mm to 0.914 mm and the sharpness index increases from 0.311 to 0.339 (see table 4, Simulations 1 and 3, X- direction) when the amount of fine particles in the mixture increases from 40% to 63% indicating on the narrow void size distribution with small voids. These trends are more pronounced for packings in X and Y directions.

3.2.2. Ternary mixtures of spherical particles and fibers. To evaluate the effect of fibers on the microstructure of powder compact, fibers (1 wt.%) were added to the mixtures of fine and coarse spherical particles. The compaction of such ternary mixtures under gravity was simulated using DEM, and the void size distributions were measured on obtained powder compacts.

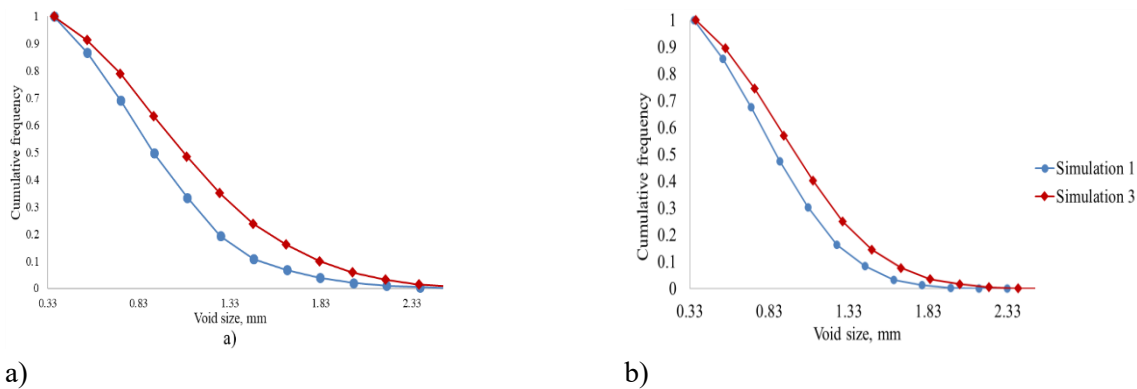


Figure 3. Cumulative frequency void-size distributions measured in (a) X, and (b) Y directions for Simulations 1 and 3.

Table 4. Parameters of void size distributions.

Parameters		d_{50}	d_{90}	d_{10}	d_{90}/d_{10}
Simulation 1 (63:37)	X	0.914	0.500	1.475	2.950
	Y	0.864	0.490	1.390	2.837
	Z	0.930	0.485	1.626	3.353
Simulation 2 (1:62:37)	X	0.940	0.528	1.530	3.211
	Y	0.900	0.500	1.457	2.944
	Z	0.795	0.437	1.268	3.109
Simulation 3 (40:60)	X	1.068	0.570	1.830	2.898
	Y	0.998	0.540	1.590	2.914
	Z	0.984	0.533	1.657	2.949
Simulation 4 (1:40:59)	X	0.960	0.540	1.550	2.870
	Y	0.965	0.540	1.515	2.806
	Z	0.870	0.475	1.380	2.905

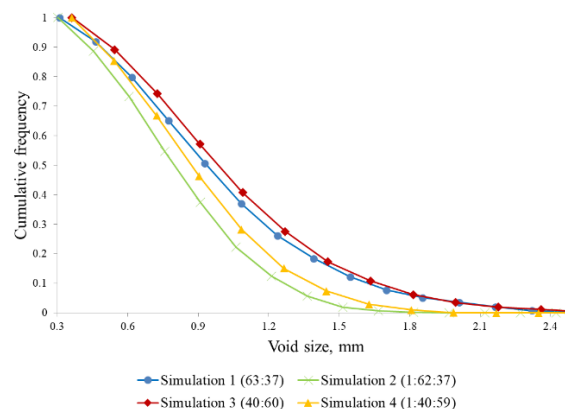


Figure 4. Cumulative frequency void-size distributions measured in Z direction for all samples.

As expected, the addition of fibers has a significant impact on the compact microstructure. The largest differences in void size distributions were observed for cross-sections normal to Z direction due to the preferential orientation of fibers, as shown in figure 4. The size of voids decreases and the distributions become sharper with an addition of fibers for both powder mixtures with low and high amounts of the fine spherical component. The densest packing with the smallest voids ($d_{50} = 0.795$ mm) and the most uniform size distribution ($x_{10} / x_{90} = 0.345$) was obtained for the ternary mixture of fibers (1%), and fine (62%) and coarse (37%) spherical particles.

4. Conclusion

The packing microstructure of powder compacts of the ternary mixture of spherical particles and fibers was investigated in the present study. The compacts of particle mixtures of various compositions were simulated using the discrete element method. The fibers were represented by the elongated ellipse-shaped particles. The particles of spherical and ellipsoidal shapes were generated using the superquadrics approach. The packings of binary mixtures of spherical particles and ternary mixtures of spherical particles and fibers were formed under gravity. The compact microstructure was characterized quantitatively by measuring the size distributions of voids among particles in X, Y and Z directions using the developed image analysis procedure. The addition of fibers resulted in denser particle packing with a more uniform distribution of smaller voids. This tendency is more pronounced for the mixture with a larger fraction of fine spherical particles. This analysis allows to evaluate incorporation of fibers on the powder compact microstructure and is useful to design the asphalt paving mixture.

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