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# Structural Characteristics of Three-Dimensional Random Packing of Aggregates with Wide Size Distribution

Kasthurirangan Gopalakrishnan and Naga Shashidhar



***Abstract*—**The mechanical properties of granular solids are dependent on the flow of stresses from one particle to another through inter-particle contact. Although some experimental methods have been used to study the inter-particle contacts in the past, preliminary work with these techniques indicated that they do not have the necessary resolution to distinguish between those contacts that transmit the load and those that do not, especially for systems with a wide distribution of particle sizes. In this research, computer simulations are used to study the nature and distribution of contacts in a compact with wide particle size distribution, representative of aggregate size distribution used in asphalt pavement construction. The packing fraction, the mean number of contacts and the distribution of contacts were studied for different scenarios. A methodology to distinguish and compute the fraction of load-bearing particles and the fraction of space-filling particles (particles that do not transmit any force) is needed for further investigation.

***Keywords*—**Computer simulation, three-dimensional particle packing, coordination number, asphalt concrete, aggregates.

## I. Introduction

THE inter-particle contacts are the path through which stresses get transmitted in granular solids [1]-[2]. The distribution and nature of these inter-particle contacts are expected to play an important role in mechanical behavior of granular solids. The parameters that affect the nature and distribution of contacts such as the particle shape and particle size distribution will be expected to affect the mechanical properties as well. Researchers have used physical methods for determining the inter-particular contact information, such as the paint method [3] and the optical techniques [4]. Preliminary work with this techniques indicated that these will not have the necessary resolution distinguish between those contacts that would be load-transmitting versus those that do not, especially for systems with a wide distribution of particle sizes. The efforts were then focused on using computer simulations to study the contact nature and distribution.

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Particle packing has both theoretical and practical importance in many areas of science and engineering. Computer simulation of particle packing is becoming increasingly attractive with the rapid increase in computing power. Particle packing simulations have been widely applied to mono-size particles [5]-[6], particles with a slight spread in sizes [7], and log-normal distributions spanning as much as 1.5 decades in sizes [8].

In some industries, it is necessary to deal with wide particle size distributions. For instance, the aggregates used in asphalt pavements typically have a 19 mm maximum size and about 5% of the particles (by weight) finer than 75 μm—a span of two and a half decades. In such cases, in order to have a representative number of large particles (25-mm particles), tens of millions of small particles have to be considered. Such simulations present significant challenges in terms of both computing requirements and algorithms to handle particles two orders of magnitude next to one another.

The study of inter-particle contacts is especially beneficial for modeling the microstructure of asphalt concrete. It is generally recognized that in asphalt pavements, the coarse aggregates form a skeleton that primarily supports the load. Shashidhar et al. [9] showed that the stress is transmitted from particle to particle through the aggregate skeleton in asphalt pavement. Using photoelastic methods, it was shown that the loads were transmitted from aggregate to aggregate in a two-dimensional representation of asphalt concrete (see Fig. 1).

The effect of the size distributions on packing characteristics of the particle have been primarily studied through physical experiments [10]-[11] and through computer simulations [2]. In areas such as ceramics and powder metallurgy, a particle system (e.g., powder) with a spread of particle sizes is closely approximated to a known size distribution and is studied by computer simulated packing of spheres. These studies have typically used log-normal or Gaussian particle size distributions with systematic variation of the standard deviation (or range of particle sizes). In these studies, it was found that the packing fraction increased when the standard deviation of the distribution increased.

In many of these studies, a rather narrow size range was considered. Nolan and Kavanagh [2] used a particle size range of 0-20, while Powell [8] used sizes from 0 to 1.0, and Bierwagen and Saunders [12] used particles of sizes from 0.1

to 10, a 2-decade range. In the systems that were of primary interest to the authors, asphalt concrete, this was not an adequate range of distribution of sizes.

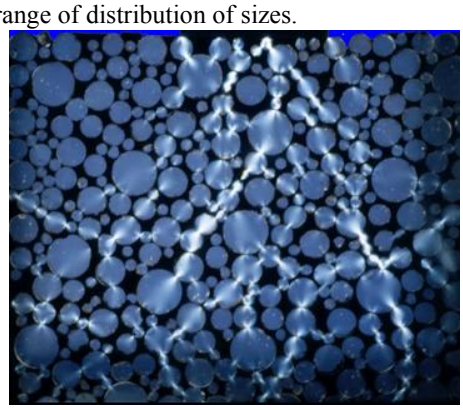

Fig. 1 Stress distribution in asphalt concrete made with glass disks replacing large aggregates (Shashidhar et al. [9])

The Discrete Element Method (DEM) [13] has been used for modeling granular systems. In order to extend the DEM techniques to real aggregates, one major step involves using a range of particle sizes. Zhong et al. [14] developed methods to use this technique for accommodating particles with sizes spanning two decades. The determination of the initial structure of the granular assembly is an important input to this modeling. The typical technique to obtain this starting assembly is particle packing simulations. Although computer simulation methods have been used extensively in modeling the microstructure of Portland cement concrete [15], their application for studying asphalt concrete is relatively new. In this paper, the nature and distribution of inter-particle contacts in computer-simulated compacts with a wide particle size range such as those found in asphalt pavements are discussed.

## II. APPROACH

Aggregates with particle size distributions that follow a simple Power law (see (1)) were considered in this paper.

$$F = \left( \frac{d}{d_{max}} \right)^k \quad (1)$$

where $d_{max}$ is the maximum particle size, d is the diameter of the sieve in question and F is the fraction finer than sieve.

A maximum particle size ($d_{max}$) of 19 mm was chosen for all the experiments since this is a popular size used in asphalt concrete. A choice of minimum size was necessary since the number of particles increase exponentially with decrease in size. The choice for the minimum particle was made by choosing values for F of 0.225, 0.25, 0.275 and 0.3. This defined the $d_{min}$ between 0.375 for (low k and low F) to 3.066 for high k and high F.

The span from $d_{min}$ to $d_{max}$ was divided into 10 logarithmically equal intervals to obtain discrete sizes for packing. The number of particles of each size was calculated and the total number was adjusted to be 80,000 particles.

## III. PACKING ALGORITHM

Computer simulation of random packing of spheres involves using an algorithm to generate the coordinates of spheres in contact [8]. The advantage of studying computer-simulated models as opposed to physical models is that the geometrical properties of the packing structure can be accurately determined, as the sphere coordinates are precisely known to the machine accuracy of the computer. This is especially invaluable in the study of granular materials as their properties are directly related to their packing geometry [16].

In this study, the packing algorithm used was similar to that of Vischer and Bolsterli [5] and Jullien and Meakin [6], in which the spheres fall under gravity sequentially and roll to their stable position. The stable position is defined as the position when the sphere rests on three contacts. The particles were dropped from random locations within the box. The algorithm included five attempts for each particle to find the lowest position, which was characterized by Vischer and Bolsterli [5] as reproducing the effect of vibration on the settling particle. The packing fraction, defined as the volume occupied by particles per unit volume of the compact, was calculated on a smaller box that was 60% of each dimension, placed centrally. This was done to avoid edge effects on the packing results. The characteristics of the packing were estimated from these reduced boxes as well.

The first step in packing simulation is to study if the packing program yields results comparable to data reported in the literature. To study this, two different studies were conducted. In the first study, 10,000 of 10-mm diameter spheres were packed in a box of dimensions 200-mm × 200-mm box. This set-up had a box size to sphere diameter ratio of 20:1. To avoid edge effects, the outer 10-mm layer of this box was cut from all sides and only the inside core was used for further analysis. Four independent simulations gave an average packing fraction of 0.5939 and a standard deviation of 0.0011. In the second experiment, 80,000 of 3-mm spheres were packed in a 120-mm × 120-mm box to yield a box size to sphere diameter of 40:1. Four independent simulations yielded an average packing fraction of 0.5940 with a standard deviation of 0.0006. By increasing the box-size to sphere diameter ratio from 20:1 to 40:1, the mean packing fraction changed a little while halving the standard deviation. These results are comparable to the values reported in the literature, which are generally in the range of 0.58 to 0.60 for monosized spheres [5]-[6].

In random packings, the coordination number need not necessarily be an integer. In most random packing studies, the distribution of coordination numbers has been found to be effective in characterizing the packing geometry and as well as in studying the structural properties of particle packings [8]. The value of the coordination number depends on the definition of nearest neighbors. In a packing of monosized spheres, the value of average coordination numbers can range from 6 to 13.4 depending on how the contacts are defined [17]. Since mechanical stresses are transmitted only when

there is good contact between spheres, the contacts are considered when L-R1-R2 <0.001 mm where L is the distance between two spheres of radius R1 and R2.

For the both the studies, the distribution of coordination numbers of the spheres was obtained. This distribution in both the studies was found to be Guassian with a mean coordination number of 6. The standard deviation for the Guassian distributions was 0.8707 showing that the distribution was narrow with very few spheres having a coordination number of 3 or 9. The maximum coordination number for these trials was found to be 9. This value is similar to the value obtained by Gotoh and Finney [18] for a dense packing.

## IV. Packing Fraction Results

As mentioned previously, there are certain difficulties in applying particle packing concepts to packing of aggregates used in asphalt concrete. To simulate the packing of aggregates in asphalt concrete, it would be necessary to pack the entire particle size distribution, which spans over 2.5 decades. This means that to represent 2 to 3 particles in coarse sizes, it is required to pack hundreds of thousands of small particles. To simplify the simulations, the particle size distributions were truncated at F = 0.30, 0.275, 0.25 and 0.275. Note that F (see Eq. 1) refers to the passing fraction as described in Eq. 1. Thus, a value of F = 0.30 means that 70% of the distribution is considered by the packing program. As F decreases, more of the particle size distribution is considered in the packing. Pictorial representation of a computer simulated packing structure obtained in this study is shown in Fig. 2.

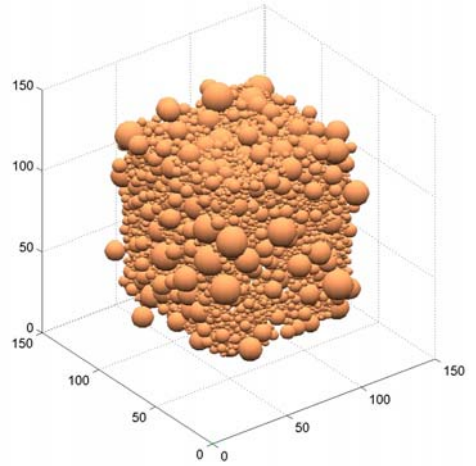


Fig. 2 Computer simulated compact with wide particle size distribution

The packing fraction is plotted as a function of F in Fig. 3. The packing fraction increases as F decreases. This observation corroborates the findings of other researchers who show a higher packing fraction as more particles are considered [5, 8].

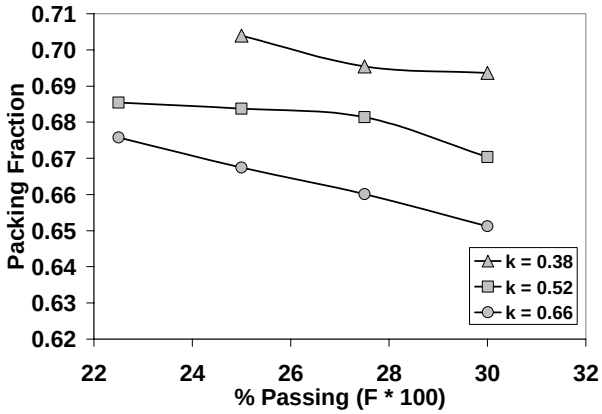


Fig. 3 Packing fraction results

For any curve in Fig. 3, say k = 0.52, a decrease in passing fraction, say from 0.275 to 0.25, which is equivalent to an increase in fractional volume of 0.025, shows only a 0.00239 increase in packing fraction. The cases, F = 0.275 and F = 0.25 at k = 0.52 correspond to minimum particle sizes of 1.587 mm and 1.321 mm, respectively. It appears that the additional volume of particles that came about in transitioning from 1.587 mm to 1.321 mm does not all go in to the interstices. If every particle went into the interstices, the packing fraction would have increased from 0.6813 to 0.6813 + 0.025 = 0.7063. But, the actual increase is only to 0.6837 indicating that these additional particles actually dilate the packing. It is thus incorrect to assume that smaller particles will all go into interstitial spaces.

Since from Eq. 1, changing F is, in effect, changes the minimum particle size, $d_{min}$, the packing fraction was plotted as a function of $d_{min}$ as shown in Fig. 4. Also, some additional cases were run for k = 0.38 and F = 0.230, 0.235, 0.240 and 0.245; and k = 0.52 and F = 0.20, 0.15 and 0.125. The plot shows that regardless of the exponent k, the packing fraction increases as $d_{min}$ is decreased until $d_{min}$ = 0.5 mm. The packing fraction then decreases fairly steeply when $d_{min}$ decreases below 0.5 mm. Also, the data is noisier at this transition zone. This behavior can either be attributed to a failure of packing algorithm to pack particles having a large size differences or a physical phenomenon that impedes the particles from packing closely. In either case, it is safe to assume that the current packing algorithm may run into difficulty when the maximum to minimum particle size ratio becomes higher than 1: 40.

Since the particle sizes have been truncated at $d_{min}$, the appropriate equation to use is as follows:

$$w = \frac{d^k - d_{\min}^k}{d_{\max}^k - d_{\min}^k} \tag{2}$$

Zheng et al. [19] showed that the exponent k is related to the packing fraction according to the following equation:

$$k = -\frac{\log \varphi}{\log R} \tag{3}$$

where φ is the packing fraction and R is a ratio of the

"coarse" and "medium" particle sizes, which is also the same as the ratio between "medium" and "fine" particle sizes.

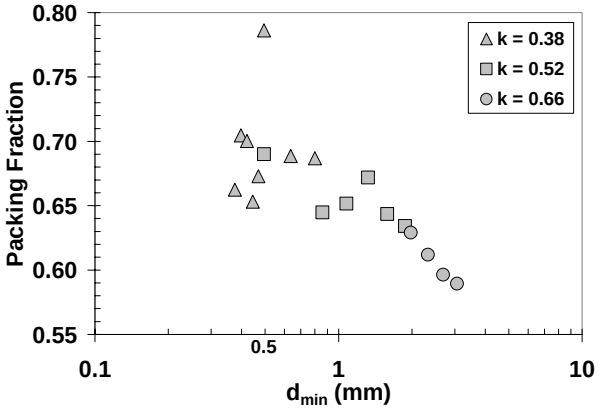


Fig. 4 Packing fraction results by minimum particle size

The designation of the different sizes of particles into "coarse", "medium" and "fine" is an outcome of the Furnas [20] model. Zheng et al. [19] considered a continuous particle size distribution as made up of several "coarse", "medium" and "fine" sets. In the context of the current study, if $d_{max}$ is defined as the "coarse" particle and the gradation is considered to be an addition of several sets of coarse, medium and fine particles, the diameter of the fine particles is expected to be slightly greater than $d_{min}$. In Fig. 5, the derivation of R is shown to be equal to $(d_{max}/d_{min})^{(1/3)}$. According to Eq. 3, a plot of log(φ) versus log(1/R) should be a straight line passing through the origin with a slope equal to k. Based on the results of the current study, Fig. 6 shows that the data does not fit this model.

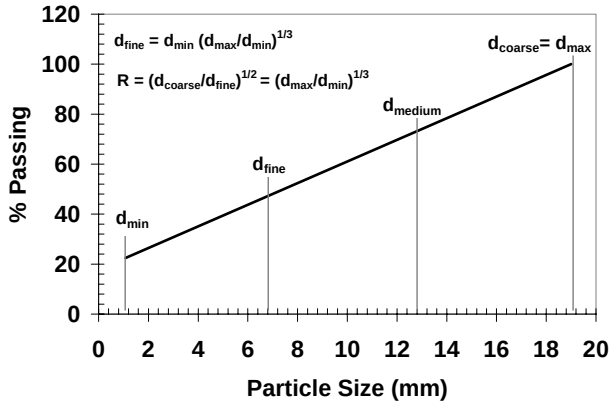


Fig. 5 Derivation of particle size ratio, R (after Zheng et al. [19])

Although Zheng et al. [19] derived the expression for k (see Eq. 3), examples to illustrate that the proposed methodology agrees with experimental results were not provided. Perhaps, a continuous distribution such as that considered in this study cannot be considered as a combination of several sets of coarse, medium and fine particles. This is because for a typical mixture of coarse, medium, and fine particles, the coarse particles will have large enough void spaces to accommodate some medium particles and the fine particles could fill the remaining voids. However, in a continuous distribution of particle sizes, the voids do not exist in quite the same way, as it would be if it were just coarse particles.

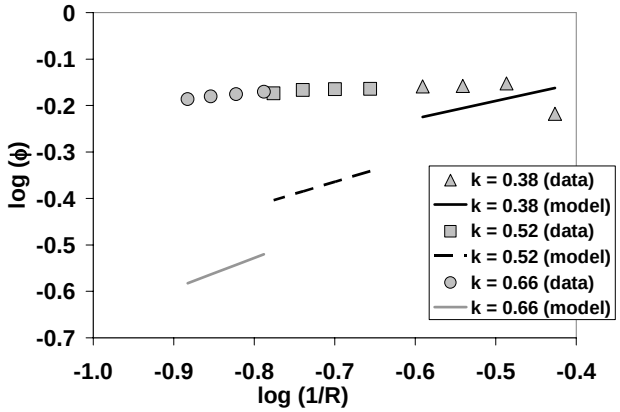


Fig. 6 log (φ) versus log (1/R) for the cases considered in this study

Other researchers have tried to extend the binary and ternary mixtures of particles to apply for continuous particle size distributions [21] based on the work done by Westman and Hugill [22]. However, the equations proposed by Westman and Hugill [22] apply only for the limiting case when the ratio of "coarse" to "medium" diameters and "medium" to "fine" diameters is infinite. In a continuous particle size distribution, the ratio between consequent sizes is hardly "infinite" and therefore the equations proposed by Westman and Hugill [22] cannot be applied. To demonstrate this, the equations proposed by Westman and Hugill [22] were actually applied to the cases considered in this study and they were not found to predict the packing fraction. The derivation is as follows:

Let us define a Class Size Ratio (CSR) which is the ratio of any two subsequent sieve (class) sizes. Then,

If Class = 1, then Fraction Passing = 1, and Fraction Retained = 0;

If Class = 2, then Fraction Passing = $(1/CSR^k) = CSR^{-k}$, and Fraction Retained = $1 - (1/CSR^k) = 1 - CSR^{-k}$;

If Class = 3, then Fraction Passing = $CSR^{-2k}$, and Fraction Retained = $CSR^{-k} - CSR^{-2k}$;

If Class = n, then Fraction Passing = $CSR^{-(n-1)k}$, and Fraction Retained = $CSR^{-(n-2)k} - CSR^{-(n-1)k}$

where $d_{max}$ is the maximum size for the distribution. The minimum size $d_{min}$ is then equal to $d_{max}/CSR^{n-1}$.

Westman and Hugill's [22] equation can be written as follows:

$$V_a = \sum_{i=1}^{n-1} x_i + a_n x_n \tag{4}$$

where $V_a$ is the porosity $(1 - \varphi)$ of the packing structure.

Now,

$$\sum_{i=1}^{n-1} x_i = (1 - CSR^{-k}) + (CSR^{-k} - CSR^{-2k}) + \ldots + (CSR^{-(n-3)k} - CSR^{-(n-2)k})$$

That is,

$$\sum_{i=1}^{n-1} x_i = (1 - CSR^{-(n-2)k}) \quad (5)$$

Therefore,

$$V_a = 1 - CSR^{-(n-2)k} + a_n (CSR^{-(n-2)k} - CSR^{-(n-1)k}) \quad (6)$$

In this study, when k = 0.38, n = 16 and CSR=1.275, and $a_n$ for the random close packing of monosize spheres is 1/0.5872 = 1.703. Using these values, we get $V_a$ = 0.767 or φ = 1.304. Since this packing fraction is unrealistic, it could be concluded that the equations proposed by Westman and Hugill [22] cannot be applied to continuous particle size distributions considered in this study.

## V. Contact Distribution Results

The particle-particle contacts are more important to evaluate the stability of the packing. The approach taken here is to measure the distribution of contacts for any given size particle. This distribution of contacts was found to be a Guassian distribution, which is similar to the distribution of contacts for random packing of monosize particles. This distribution normalized by the total number of particles of that size is plotted in Fig. 7.

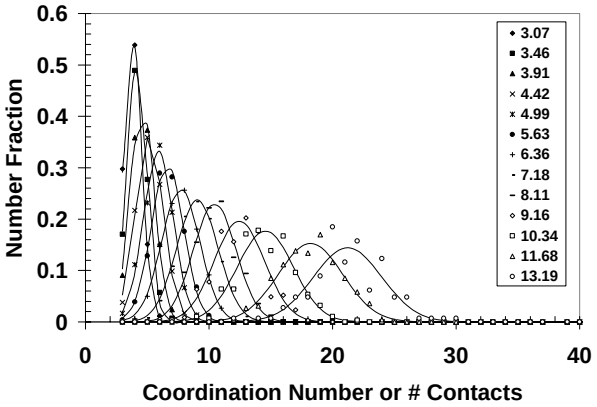


Fig. 7 Distribution of contacts

Several observations can be made from Fig. 7. The distributions of contacts are narrow for smaller size particles and broad for larger size particles. The mean number of contacts increases as the particle size increases. In other words, the larger the particle size, the more contacts it is likely to have. The data tends to get noisier as the particle size increases. The reason for this is that there are fewer larger particles than there are smaller particles. Therefore, the smaller sizes have better statistics than larger particles. The larger particles have a wider range of number of contacts. This is because the size of the particles in contact with a give particle dictates how many particles can be in contact. A particle can have many smaller particles contacting it or fewer larger particles touching it.

Each of these distributions was characterized using a Gaussian distribution function and the mean and standard deviations were estimated. The regression results were excellent with $R^2$ greater than 0.99 for smaller particles. However, as the particle size increased, the noise in the data caused poorer fits and curves with lower $R^2$ values were not considered for further analysis.

In Figs. 8 and 9, the mean and standard deviations of the Gaussian curves are plotted as a function of the particle size (d). When the mean and standard deviations were normalized by the minimum particle size ($d_{min}$), the individual curves collapsed into a single master curve in each case. The results are shown in Figs. 10 and 11. A quadratic equation could be fit for each of the master curves (one for mean and one for standard deviation). The following equations for mean and standard deviation represented the data well:

$$Mean = A + B\left(\frac{d}{d_{\min}}\right) + C\left(\frac{d}{d_{\min}}\right)^2 \quad (7)$$

$$S\tan dard\ Deviation = D + E\left(\frac{d}{d_{\min}}\right) + G\left(\frac{d}{d_{\min}}\right)^2 \quad (8)$$

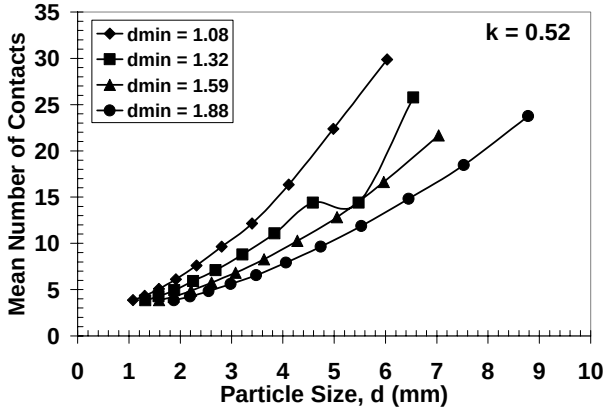


Fig. 8 Mean number of contacts versus particle size

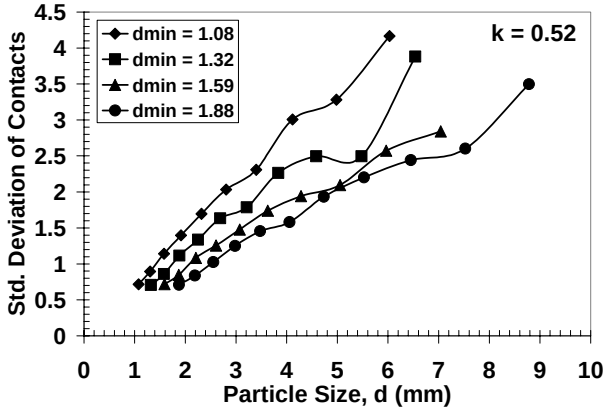


Fig. 9 Standard deviation of contacts versus particle size

The $R^2$ for these second-order polynomial regression equations were greater than 0.97 indicating good fits. The coefficients A-G for these fits are displayed in Table 1. This approach can be used to compare different particle size distributions, or aggregate gradations in the case of asphalt pavement mixtures, as shown in Figs. 12 and 13. These plots

show that particle size gradation influences the mean number of contacts to some extent and the standard deviation of contacts to a large extent. For a given particle size diameter, the higher k-value has a lower standard deviation. The mean number of particles is almost independent of k-value.

TABLE I
REGRESSION ANALYSIS RESULTS

| Regression Model Coefficients | k = 0.38 | k = 0.52 | k = 0.66 |
|---|---|---|---|
| A | 2.054853 | 2.002355 | 1.655982 |
| B | 1.075094 | 1.12836 | 1.336999 |
| C | 0.739957 | 0.696957 | 0.718803 |
| D | -0.27737 | 0.019299 | 0.03865 |
| E | 1.019175 | 0.763897 | 0.725217 |
| G | -0.00372 | -0.01366 | -0.01691 |

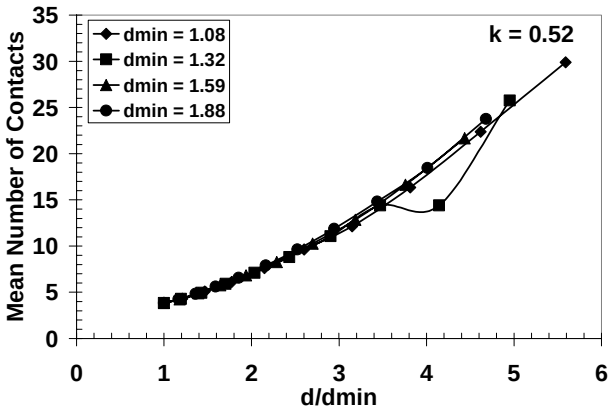


Fig. 10 Mean number of contacts versus $d/d_{min}$

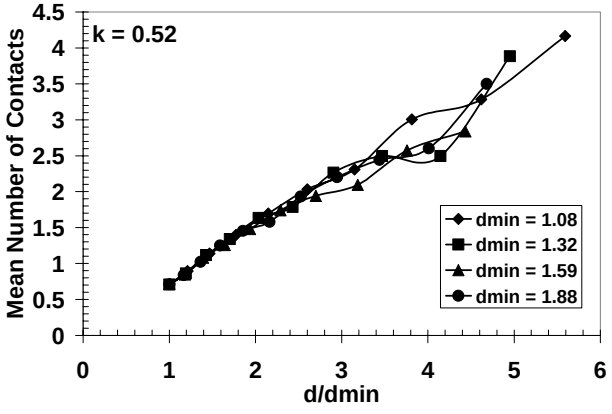


Fig. 11 Standard deviation of contacts versus $d/d_{min}$

In a different experiment, particles with a lower maximum size ($d_{max}$) of 13.3 mm was repeated since these maximum sizes represent one of the typical particle size distributions used in asphalt pavements. The maximum size also matches the experiments for which the physical results have been obtained previously [23]. The results were very similar to those shown in Figs. 7 to 11. Thus, the behavior of contact distribution is independent of the maximum particle size ($d_{max}$).

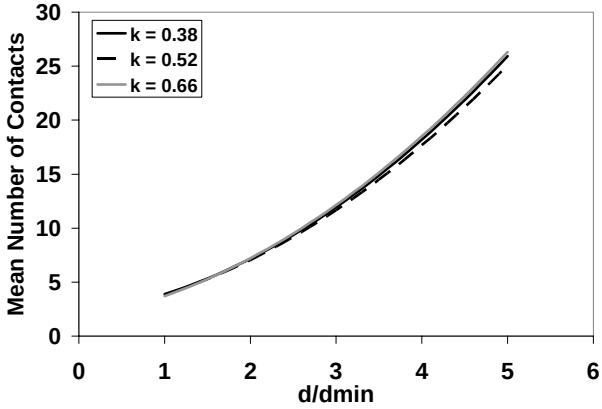


Fig. 12 Comparison of contact distribution statistics for different gradations (mean)

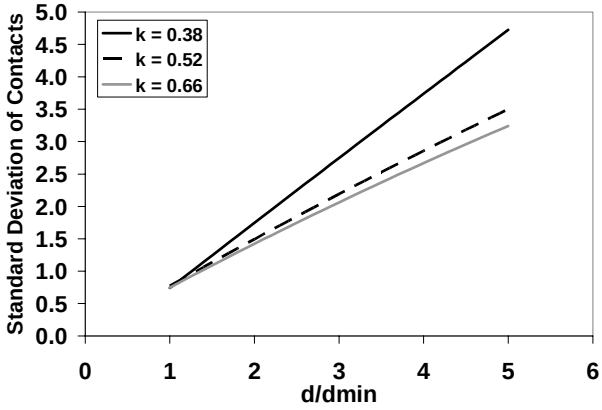


Fig. 13 Comparison of contact distribution statistics for different gradations (standard deviation)

The distribution of contacts for a given particle size is consistent with the observation for monosize particles. Equations (7) and (8) that describe the master-curves for contacts contain lot of useful information. Due to current computational limitations, the packing program could only pack to a minimum size of 1.08 mm for k = 0.52 gradation. With these master-curves it would be possible to estimate what the number of contacts would be if the gradation were packed down to smaller size particles. For instance, if a powder with maximum size of 19 mm and a minimum size of 0.075 mm were packed, a 2.36 mm particle would have a mean number of contacts of 728 and a standard deviation of 10.53. This certainly is a large number of contacts. The mechanical properties of the packing are dependent on how many of these contacts actually transmit force when the packed assembly is stressed. Travers et al. [24] showed through photo-elastic experiments on a two dimensional

packing of cylinders that only two or three contacts seemed to transmit load even though there seemed to be six contacts on an average. It is therefore necessary to come up with an additional criterion to define load-transmitting contacts.

Consider Fig. 14, which is a close-up of a likely scenario in a two dimensional packing assembly. When this assembly of particles is stressed, the most likely situation is that the force will travel through a path that will bypass the small particles. In other words, the contact must be a stable part of a skeleton for the stress to pass through it. If we consider all the particles that form such a stable skeleton to be load-bearing, then there has to be some criteria to classify the load-bearing particles. Future studies will focus on deriving such a criterion to divide a particle as load-bearing or non-load bearing.

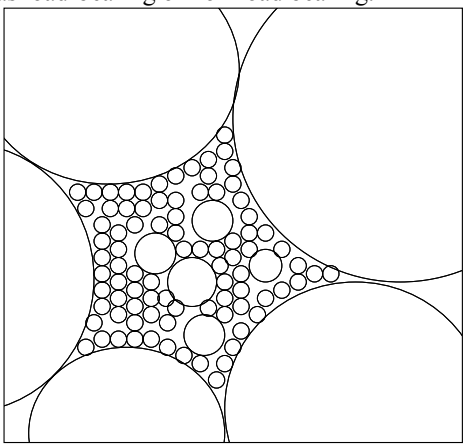

Fig. 14 A schematic of 2D packing assembly of particles

Shashidhar et al. [9] demonstrated that asphalt concrete behaves more like a granular system and have shown the possibility of developing a relationship between the aggregate structure and asphalt pavement performance through micro-mechanics based modeling and image processing techniques. The knowledge of the relationship between the aggregate structure and the mechanical properties will enable one to engineer pavements to have the appropriate aggregate structure to maximize the field performance.

The results from this current study, especially the contact distribution characteristics, together with the principles of granular mechanics, could be used in understanding the transmission of load through aggregate contacts.

## VI. Conclusions

A stable random close packing of particles having a size distribution was modeled by applying the concepts of particle packing simulations. The packing density and the coordination number were studied.

The packing fraction of the packing increases as smaller particles are considered until a critical size. When sizes below this critical size are considered, the packing fraction decreases with particle size. The small particles can be considered to (a) fill up small spaces which tend to increase the packing density and (b) dilate the structure, which will decrease the packing density. As the minimum particle size is decreased, the competition between the two mechanisms seems to yield a critical particle size that gives the maximum packing. This critical size was found to be dependent on the particle size distribution.

A continuous particle size distribution cannot be approximated as a sum of several "Furnas sets" of coarse, medium and fine particles.

The coordination number of any size particles in the packing of particles with a continuous size distribution was found to be a Guassian distribution whose mean and standard deviation can be estimated. The mean number of contacts and the standard deviation of this distribution increased with particle size. Regression equations were developed to predict the mean and standard deviations of contacts in simulated packing structures.

The contacts can be distinguished between those that are likely to transmit load and those that are not likely to transmit load according to the coordination number of the particle it is touching. Future research efforts will focus on deriving such a criterion.

The application of particle packing simulation concepts discussed in this paper to the study of aggregate structure in asphalt pavements, in conjunction with the recent advances in nondestructive imaging techniques and DEM simulations have tremendous potential to help us to develop a deeper understanding of the aggregate structure in asphalt concrete, develop and optimize the various parameters that describe the aggregate structure and relate them to the performance of pavements in a scientific way. This will provide the foundations to building more durable and long-lasting pavements.

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