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Modeling of asphalt mixture based on aggregate morphology distribution using the contact dynamics method

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ABSTRACT: Asphalt mixture performance depends highly on the particle shape. Discrete element method (DEM) has become a highly prevalent approach for testing and reconfiguring particles in asphalt mixtures in recent decades. Nevertheless, most simulation studies simplify particle shapes and ignore irregular morphology features. In this study, morphological characteristics for a large number of particles were analyzed statistically using three-dimensional laser scanning technology. Combining morphology statistics and particle size distribution, numerical samples of asphalt mixtures were generated using Voronoi tessellations. Finally, the model reliability is validated by conducting experiments and simulations for the complex modulus test based on the Contact Dynamics (CD) method. Using this procedure, the aggregate morphology and size distribution can be incorporated in numerical simulations of asphalt mixtures. The modeling method provides a basis for the high-precision simulation of asphalt mixes comprising polyhedral particles, which can be seen as an enriching improvement of the classical procedures.

Keywords: Morphology characterization, Contact dynamics Method, 3D laser scanning, Particle tessellation, Complex modulus

1 INTRODUCTION

Asphalt mixture is an integral component of pavement materials. It includes aggregate particles enclosed by a viscoelastic matrix made up of bitumen, filler, and air. Hence, the mechanical behavior of this multiphase material is highly dependent upon the properties of the interacting components.

In the last few decades, discrete element method (DEM) has proven effective for simulating granular materials at the particle-scale. As the morphology of aggregate particles has an essential influence on the mixture performance (Chen et al., 2013; Souza et al., 2012; Castillo et al., 2018; Zhou et al., 2019; Quezada-Guajardo & Chazallon, 2021), establishing a numerical model closer to real particle assembly is an issue that deserves much attention. Many studies are currently being conducted on the simulation of irregular particles using computer-assisted algorithms (Lu & McDowell, 2007; Ma et al., 2018; Zhou et al., 2018) and image scanning devices (Tutumluur et al., 2012; Liu et al., 2017; Li et al., 2020). Despite this, most studies modeled particles as clumps of spheres, entirely ignoring important particle properties like angularity. As a result, granular fabric properties are more or less impacted, including porosity, contact anisotropy, and force chains (Alonso-Marroquin & Herrmann, 2002; Azéma

et al., 2009). Although high-resolution particle clumps can capture the characteristics of real particles, their enormous computation costs are unaffordable. Moreover, current numerical models only treat the aggregate size distribution explicitly, particle shapes used in the current research are usually created or selected randomly in the simulation and do not consider the aggregate morphology distribution in the real assembly. Selecting limited particle templates is not representative of real samples due to the wide variation of particle shapes in nature. Additionally, preparing numerical samples consisting of polyhedral particles is a very time-consuming process. During the preparation stages, such as gravity deposition, compaction, and stabilization of numerical samples, complex algorithms are required for contact detection and repulsive force computation.

In this study, the morphological characteristics of a significant number of particles were analyzed statistically based on the acquisition of three-dimensional (3D) aggregate shapes from laser scanning. The contact dynamics (CD) method is introduced to simulate irregular particles, and numerical specimens of asphalt mixtures were generated by a tessellation method based on aggregate size distribution and morphology data. Numerical and experimental tests were conducted on the complex modulus to verify model reliability at different temperatures and loading frequencies. The modeling method presented in this study is founded to provide a basis for establishing high-precision asphalt mixture models and optimal pavement design.

2 AGGREGATE SHAPE STATISTICS

2.1 Statistical distribution of particle aspect ratio

During this study, aggregate particles with sieving sizes ranging from 4 mm to 31.5 mm were selected from the stockyard. A portable three-dimensional laser scanner (FARO Edge ScanArm HD) was adopted to obtain real geometrical data of the selected 500 aggregates. After scanning and acquiring data from all specimens, the point cloud data obtained by the laser scanner was imported into MATLAB for further processing, as illustrated in Figure 1. Particle dimension characteristics are described by the ratio of their three linear dimensions, length (L), width (I), and thickness (S). Depending on whether a particle resembles a column or a plate, the Elongation ratio (LI) and Flatness ratio (IS) are determined. If the value of LI and IS is closer to 1, the aggregate is nearer to a cube. Otherwise, particles are more elongated or flatted. The minimum bounding box algorithm (Ge et al., 2018) was used to calculate the dimension values of L, I, and S of a particle.

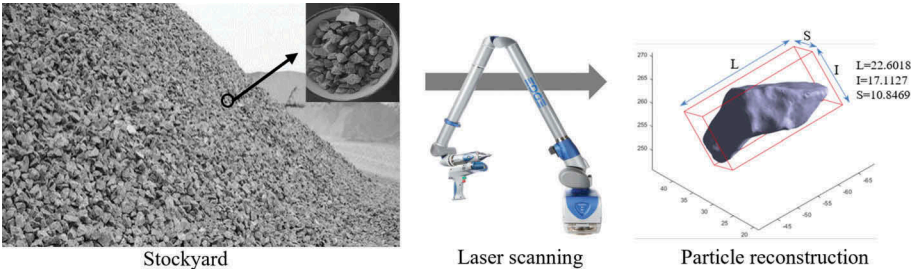
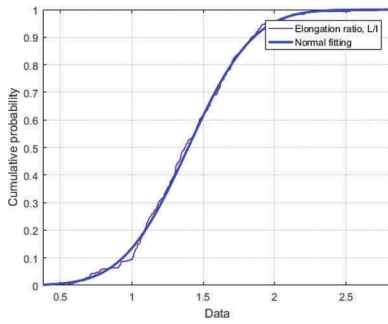
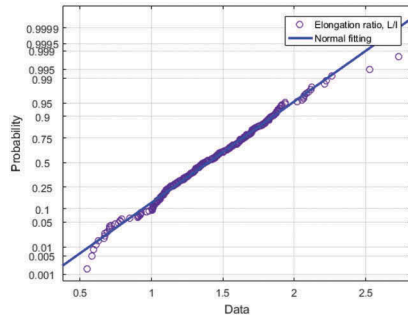


Figure 1. Materials preparation and laser scanning of particles.

Statistical features of LI and IS of all particles were analyzed. Figure 2 and Figure 3 show the Cumulative distribution histogram (CDF) and normal P-P plot of the LI and IS, respectively. The normal P-P plot is used to test if the data follows the normal distribution. As shown in the figures, the LI and IS of aggregate particles both obey the normal distribution.

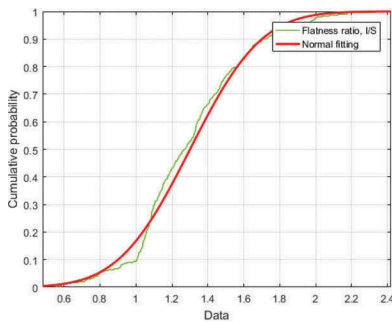


(a) LI-CDF

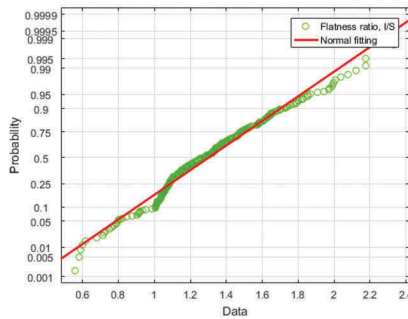


(b) LI-PP

Figure 2. LI statistics.



(a) IS-CDF

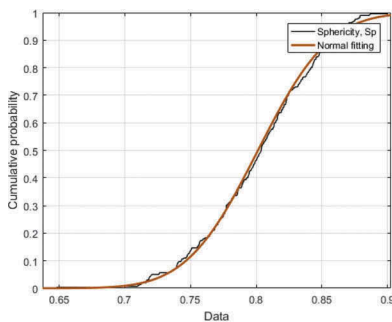


(b) IS-PP

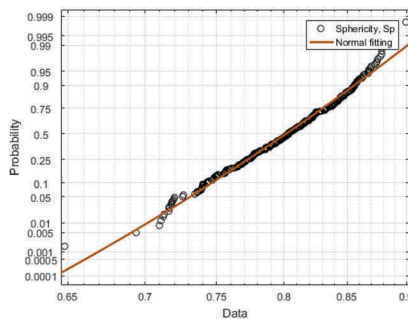
Figure 3. IS statistics.

2.2 Statistical distribution of particle angularity

Angularity belongs to mesoscopic shape characteristics. If particles are closer to cubes and their edges are sharper, it will be more favorable to the mixture interlocking. If aggregates are rounded, the overall mixture strength will be significantly reduced, even with better gradation. The Sphericity value ($Sp = \sqrt[3]{36\pi V^2/A}$) was used to characterize the angularity of aggregate particles, here, V and A represent particle volume and surface area, respectively. The closer this value to 1, the more spherical a particle.



(a) Sphericity-CDF



(b) Sphericity-PP

Figure 4. Sphericity statistics.

The statistics of Sp were analyzed using the same method above, as Figure 4 displays. The results show that the Sp obeys the normal distribution approximately. The average aspect ratio (L: I: S) for aggregates is about 1.815: 1.301: 1, the mean and standard deviation of the Sp are 0.8013 and 0.0428 respectively.

3 MODELING PREPARATION

3.1 Contact dynamics method

Discrete element method (DEM) is an approach dedicated to analyzing the assembly behavior of interacting particles. In the contact dynamics (CD) method, the contacting laws are non-differential steep laws defining the relation between relative velocities \mathcal{V} and impulses I . A significant advantage of the CD method is that particle dynamics determine the characteristic system time, so a larger time step than that in the explicit DEM method can be used. The CD method was adopted as our simulation strategy for modeling asphalt mixture consisting of polyhedral aggregate particles because of its advantages. The open-source software LMGC90 (https://git-xen.lmgc.univ-montp2.fr/lmgc90/lmgc90_user/-/wikis/home) is adopted in which CD method is completely implemented.

3.2 Numerical modeling of irregular aggregates

Asphalt mixture is composited by two main types of material: aggregates and asphalt mastic, where aggregates occupy almost 95% mass in the mix. Consequently, asphalt mixture can be seen as a system of irregular particle tessellations from a geometrical point of view, and particles interact with each other through asphalt mastic between them. Therefore, the open-source software NEPER (Quey et al., 2011; Quey & Renversade, 2018) is adopted to generate particle tessellation samples.

The viscoelastic behavior of an asphalt mixture under cyclic loading can be assessed by the dynamic modulus $|E^*|$ and the phase angle Φ . To identify the mechanical properties of asphalt mixtures, complex modulus tests were conducted in a two-point bending (2PB) configuration according to the EN 12697-26:2012 specifications (EN et al., 2012).

Table 1. Particle size distribution (PSD) of asphalt mixture.

Diameter (mm)	12.5	10	8	6.3	4	2	1	0.5	0.25	0.125	0.063
PSD (%)	100	90	75	58	44	31	20	15	12	9	6.5

Two main parameters need to be input before generating a trapezoidal numerical specimen for the 2PB test. For particle size, aggregate size from the PSD results (Table 1) was inputted to simulate aggregate gradation. For particle morphology, the aspect ratio, sphericity, and distribution of the aggregate shape parameters from the previous statistics were inputted into the NEPER software. In this way, aggregate morphology and aggregate size can be incorporated into numerical simulations of asphalt mixtures.

After the generation, about 5,680 tessellations were created following the experimental gradation cut at 2 mm to reduce the total quantity of elements in the sample, in which finer aggregates are included in the asphalt mastic. Then, the vertices of each tessellation were imported in LMGC90 to build numerical models. In this stage, particles were generated based on the convex hull of vertices from the tessellation. As rigid particles interact with each other through viscoelastic asphalt mastic between them, the particle size is decreased by multiplying a correction factor (Gaillard et al., 2020) to create gaps among particles to model the mastic, Figure 5 displays the snapshot of the numerical sample reconstructed in LMGC90 software.

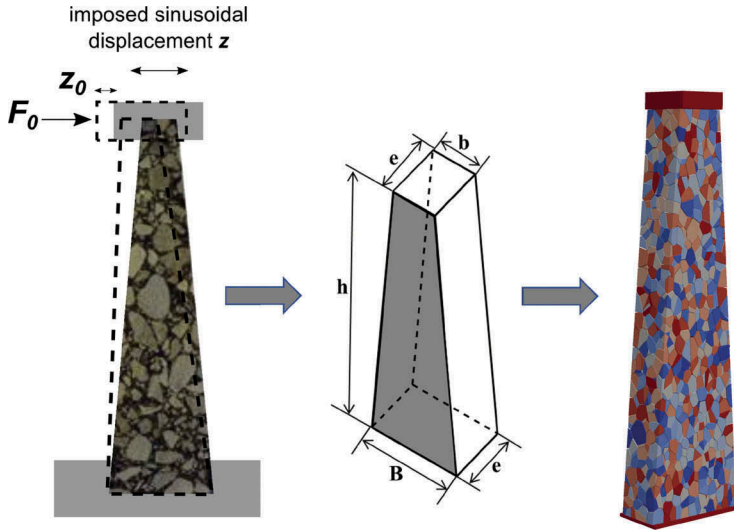


Figure 5. Test set-up and numerical modeling of test sample.

4 NUMERICAL MODELING VALIDATION

4.1 Calibration of the Burgers model

Asphalt mixture is a complex composite material showing a viscoelastic behavior, thus a viscoelastic contact model based on the Burgers model is adopted in the simulation. This model comprises a Maxwell model putting in series with a Kelvin-Voigt model (Figure 6), the stiffness and the viscosities for the Maxwell and the Kelvin-Voigt parts correspond to K_m , C_m , K_k , and C_k , respectively. More details about the numerical implementation of this contact model can be found in (Quezada & Chazallon, 2020).

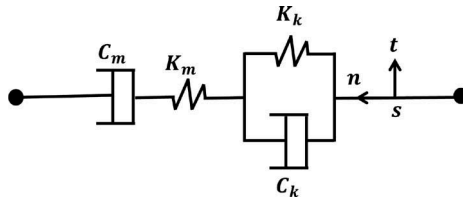


Figure 6. Burgers contact model between particles.

For a viscoelastic material under cyclic loading, it is possible to determine the complex compliance from the resulting strain and stress as following:

$$|D^*| = \sqrt{D'(\omega)^2 + D''(\omega)^2} \quad (1)$$

$$D'(\omega) = \frac{1}{K_m} + \frac{K_k}{K_k^2 + \omega^2 C_k^2} \quad (2)$$

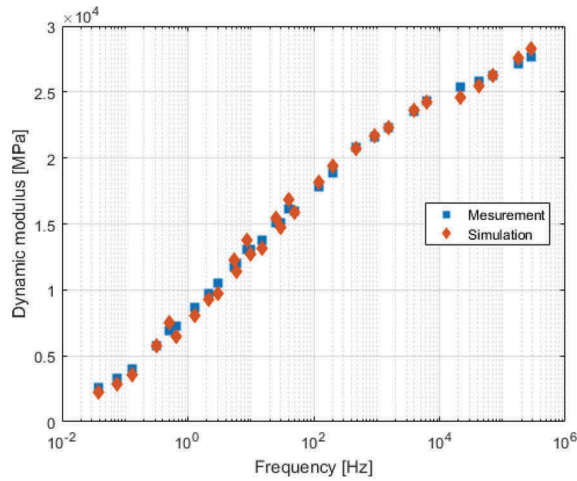
$$D''(\omega) = \frac{1}{\omega C_m} + \frac{\omega C_k}{K_k^2 + \omega^2 C_k^2} \quad (3)$$

Where:

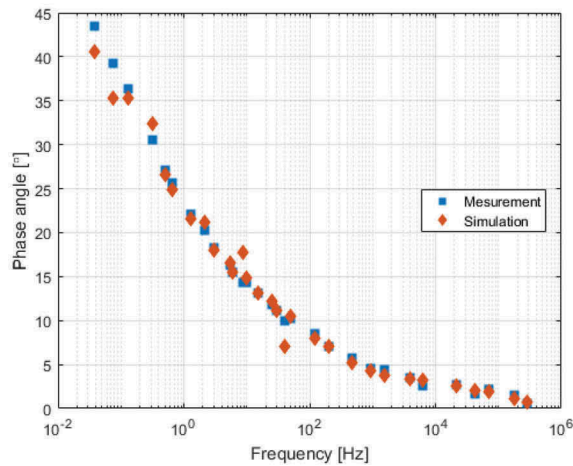
- K_m, C_m, K_k and C_k correspond to the Maxwell and Kelvin-Voigt stiffness and viscosities respectively.
- $|D^*|$ is the complex compliance, D' and D'' are the real and the imaginary parts of the complex compliance, and ω is the pulsation.

4.2 Macro mechanical behavior

The master curve describing the loading time dependency of asphalt mixtures can be generated according to the time-temperature superposition principle. To build the corresponding master curve, a reference temperature T_{ref} was chosen, then the translation of all isotherm values was performed by calculating the reduced frequency as $f_r = a_T \times f$, where f corresponds to each frequency value in each curve and a_T is the shift factor. These values are obtained from the temperature fit using the Williams-Landel-Ferry (WLF) equation (Eq. 9):



(a) Dynamic modulus



(b) Phase angle

Figure 7. Experimental and numerical master curve at $T_{ref} = 15^\circ\text{C}$.

$$\log a_T = \frac{-C_1(T - T_{ref})}{C_2 + (T - T_{ref})} \quad (4)$$

Where:

- C1 and C2 are 28 and 206.8 °C respectively, and T is the test temperature.

Figure 7 Displays the experimental and numerical results for the master curve at the reference temperature of 15 °C, which is a referenced value in French pavement design (EN et al., 2012).

The numerical values from simulations are in good agreement with experimental values for $|E^*|$ and Φ for all the tested frequencies, despite some fluctuations around the average values. The best fitting parameters for the Burgers contact model are listed in Table 2.

Table 2. Burgers model parameters used in numerical simulations.

T (°C)	K_m (Pa)	C_m (Pa.s)	K_k (Pa)	C_k (Pa.s)
-10	1.34×10^8	1.79×10^8	2.55×10^9	3.26×10^7
0	1.18×10^8	6.86×10^7	9.36×10^8	1.03×10^7
10	1.02×10^8	1.93×10^7	2.80×10^8	3.05×10^6
15	9.48×10^7	1.02×10^7	1.70×10^8	1.79×10^6
20	8.64×10^8	4.81×10^6	1.02×10^8	1.05×10^6
30	7.18×10^7	8.84×10^5	3.39×10^7	2.80×10^5

4.3 Particle movement characteristics

During the 2PB test, a trapezoidal sample is fixed between two plates, and a sinusoidal displacement is applied to the top of the sample, while the bottom base remains fixed. Empirically, the macroscopic fracture usually occurs at 1/3 sample height from the bottom, as figure 8 (left) shows. To conduct the microanalysis at the particle level, a particle is selected at the critical position (side center of the 1/3 sample height) and its displacement during one loading cycle is recorded and shown in figure 8 (right). As can be seen, the displacement is mainly a result of horizontal particle movement. Besides, similar results have been found for the particle located at the left part of the sample. The peak value of particle displacement magnitude was chosen and its changing trend was further analyzed under different temperatures and frequencies. Figure 9a shows that particle displacement increases with the temperature, and the displacement increases especially dramatically above the temperature exceeds 20 °C.

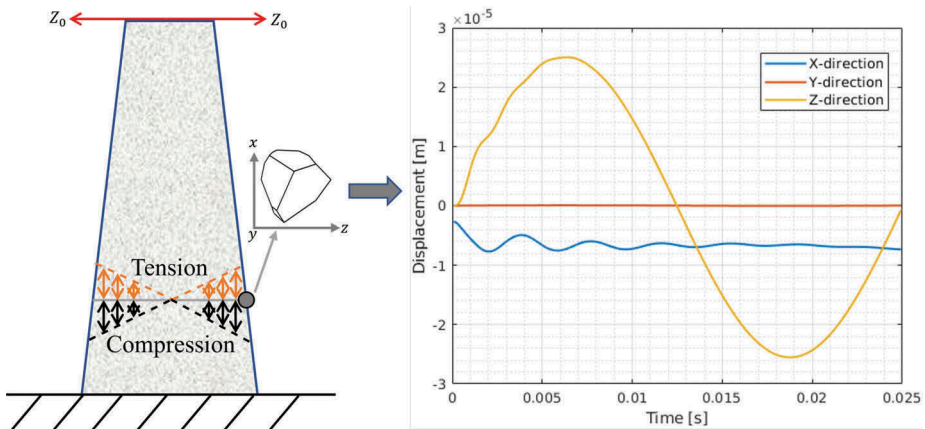
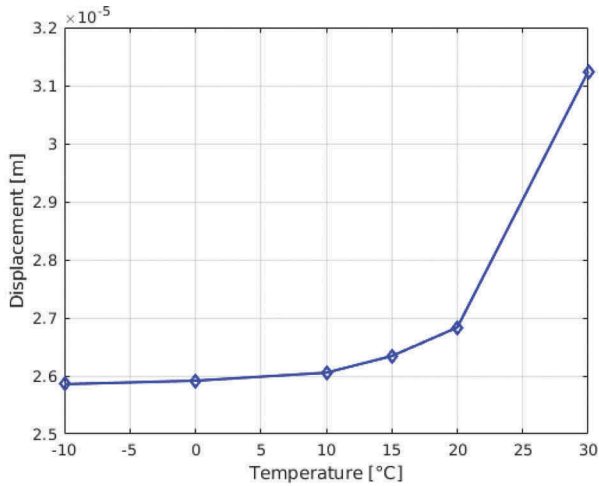
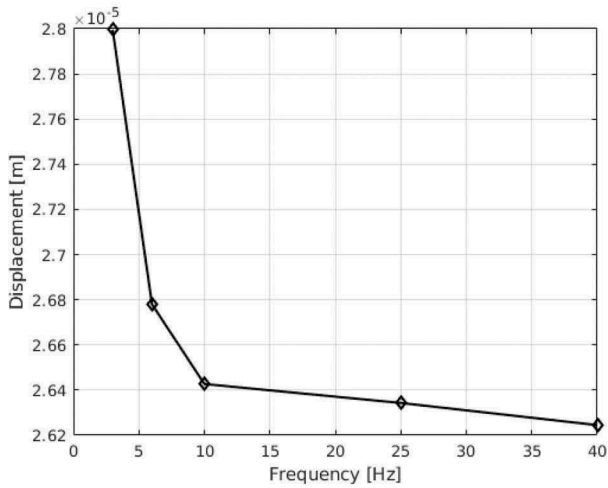


Figure 8. Macro-mechanical behavior and displacement distribution for the particle located at the third height (right) of the sample.



(a)



(b)

Figure 9. Maximum particle displacement under different (a) temperatures (b) frequencies.

According to Figure 9b, particle displacement decreases with increasing frequency, and its decrease becomes dramatic as frequency exceeds 3 Hz. The above results indicate that asphalt mixtures are sensitive to temperature and loading frequency due to their viscoelastic nature, especially at low frequencies and high temperatures. Furthermore, it also reveals that a test sample at high temperatures or low loading frequencies tends to produce significant particle movements, which could cause large bending deformations at the macroscopic level. Additionally, the results confirm the frequency–temperature superposition where the large displacement corresponds to high-temperature and low-frequency.

5 CONCLUSION

In this study, laser scanning technique was combined with image processing to statistically analyze the morphology features of aggregates. Aggregate flatness ratio, elongation ratio, and

Sphericity value all obey normal distribution approximately. The obtained statistical parameters were then used as input particle shape parameters in the numerical simulation. The 2PB specimens of asphalt mixtures were created using a tessellation method based on particle morphology statistics and then simulated in the discrete element framework based on the CD theory. With regard to the master curves, these simulations were in good agreement with experimental findings. The modeling method presented in this study incorporates aggregate morphology and size distribution in the numerical simulation, which provides a basis for the high-precision simulation of asphalt mixtures. Additionally, the micro-mechanism of mixture damage can be revealed at the particle level by using the proposed method.

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