Numerical Simulation of HMA Compaction Using Discrete Element Method

Jingsong Chen, Graduate Research Assistant
Department of Civil and Environmental Engineering, The University of Tennessee, Knoxville, TN, USA
Department of Geotechnical Engineering, Tongji University, Shanghai 200092, P.R. China

Baoshan Huang, Associate Professor (corresponding author)
Department of Civil and Environmental Engineering, The University of Tennessee, Knoxville, TN, USA

Xiang Shu, Postdoctoral Research Associate
Department of Civil and Environmental Engineering, The University of Tennessee, Knoxville, TN, USA

ABSTRACT: Aggregates gradation and structure play an important role in asphalt concrete and are primarily responsible for resisting many types of pavement distress. In order to obtain a well-designed HMA mixture, aggregate should be well-proportioned to form a stable skeleton and provide sufficient void space to fill in asphalt cement. However, in traditional asphalt mix design, it is highly dependent on engineers' experience to select a good aggregate blend and the process is time-consuming and requires significant human and materials resources. In this study, discrete element method (DEM) was used to simulate the compaction of hot-mix asphalt (HMA) with the Superpave gyratory compactor (SGC). The open source DEM code, YADE, was modified and implemented with the C++ programming language to simulate SGC compaction. The viscoelastic properties were considered through Burger's contact model, and the input parameters were calibrated from dynamic modulus test results by nonlinear regression. Five different aggregate gradations were simulated. The results show that DEM is an effective tool to simulate asphalt mixture compaction and may be very helpful for asphalt mixture design.

KEY WORDS: Discrete Element Method, Superpave Gyratory Compaction, Open Source Code, Burger's Model

1 INTRODUCTION

Hot-mix asphalt (HMA) is a multi-phase composite material which consists of asphalt binder, coarse aggregate, fine aggregate, mineral filler, and other additives. In a typical HMA mixture, aggregate accounts for approximately 80 percent of its overall volume or even higher. Aggregate gradation and structure play a critical role in the performance of hot-mix asphalt (HMA). A well-designed HMA mixtures must have a strong aggregate skeleton to sustain and pass traffic loads to the underlying layers and the voids in mineral aggregate (VMA) are required to be sufficiently high to accommodate appropriate amount of asphalt content and air voids (Roberts et al. 1996).

Many researchers have proposed various ways to improve the performance of asphalt mixtures through optimizing aggregate gradation and structure (Roque et al. 1997, Birgisson and Ruth 2001). Among these ways, the Bailey method has been getting more and more attention and been successfully used in the selection of proper aggregate gradation. The Bailey method was originally developed by Robert Bailey from the Illinois Department of Transpiration in the early 1980s. It is a systematic approach to selecting and adjusting aggregate gradation in HMA for a strong skeleton for rutting resistance along with adequate VMA for good durability (Vavrik et al. 2001, 2002). However, Bailey method is a semi-empirical model and the whole procedure is a complicated calculating and revising process which is rather time consuming.

Discrete element method (DEM) is a newly developed numerical method in recent decades and was first proposed by Cundall (1971). Due to the advantage of simulating the deformation process of joint system or discrete particles assembly, discrete element method was widely used in the fields of geotechnics, mechanics, chemistry, astrophysics etc (Ting 1989, Jing 2000, Xie 2009). The application of DEM in asphalt concrete was relatively late (Meegoda 1993, 1994). With the development of computer technology, DEM has been more frequently employed to study the mechanical behavior of asphalt mixtures. Kim (2005) used DEM study the fracture of asphalt concrete. You (2004) and Adhikari (2008) predicted the modulus or dynamic model of asphalt concrete by using discrete element modeling approach. The viscoelastic behavior of asphalt mixtures was also studied by using discrete-element method (Meegoda 1994, Liu 2007, Abbas 2007). Wang (2007) investigated the influence of particle shape and binder stiffness on compaction of pavement material by using PFC-3D, but the whole compaction process was not studied.

The objective of this paper is to simulate Superpave gyratory compaction process by using an open source DEM code, YADE. The viscoelastic properties was considered by using Burger’s contact model, and the input parameters were obtained from dynamic modulus test results through nonlinear regression method. The scope of this study included the calibration of Burger’s model parameters through statistical regression of dynamic modulus test results for asphalt mastics and the DEM simulation of SGC compaction of five different aggregate gradations.

2 DISCRETE ELEMENT METHOD AND YADE CODE

Discrete Element Method is a powerful numerical tool for computing the motion of a large number of particles such as granular materials. In DEM all particles are assumed to be rigid bodies and the interactions only happen at contacts or interfaces between these bodies. Behavior at the contacts uses a soft-contact approach and rigid particles are allowed to overlap one another at contact points. According to the force-displacement law, the overlap in every contact will generate interaction force between particles. A set of contact forces acting on the particle and the external stresses (like gravity) will cause the motion of particles which is calculated by the Newton’s second law. The motion of particles consequently changes the contact situation and results in the changes of contact forces between particles, which continually bring about new motion of particles.

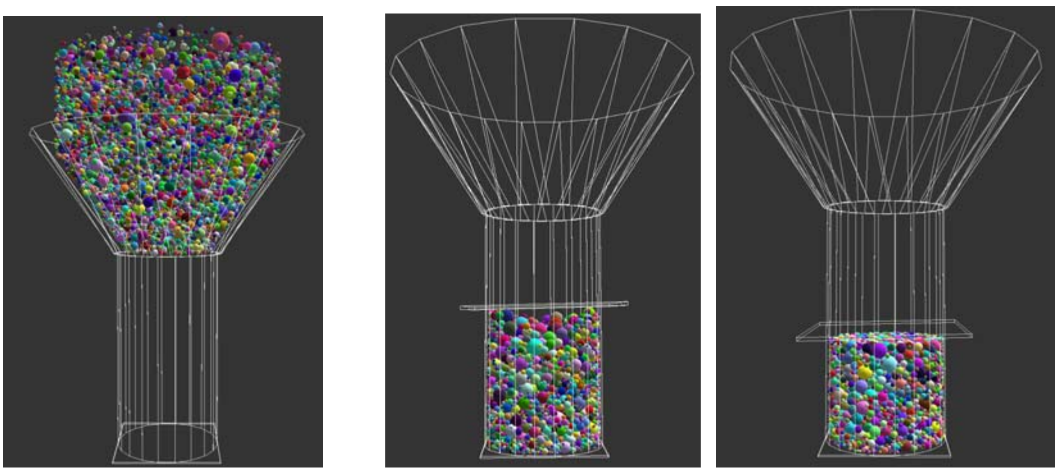
DEM code plays a very important role in the research and application of discrete element method. One of the commonly used DEM software is Itasca software PFC2D and 3D, both widely used in particle materials analysis. In this paper, an open source DEM code YADE was modified to conduct virtual SGC compaction. YADE Open-DEM is an Open Source GNU/GPL Software framework designed with dynamic libraries and implemented in C++ language. It provides a stable and uniform environment for researchers to implement computational algorithms for DEM and allows easy code reuse, exchange and extensibility (Chen 2007, Kozickij 2008).

3 MODELING AND SIMULATION PROCESS

Due to the limitation of computer processing capability, only aggregates greater than 2.36mm were considered in the DEM simulation. In fact, coarse aggregates compose the skeleton structure of asphalt mixture, undertake the main traffic load and have significant influence on mechanical behavior of asphalt mixture (Pan et al. 2005, Huang et al. 2009). The main role of fine aggregate is to fill the voids between coarse aggregates and increase the density of asphalt mixture. In this study, the fine aggregates and asphalt binder were assumed to be mixed together as special mastic which was considered by the contact constitutive law between coarse aggregates and the coarse aggregates were assumed to be spherical balls wrapped with asphalt mastic.

The whole asphalt mixture packing process was simulated as Superpave gyratory compaction process. In this simulation, the vertical pressure was set at 600 kPa and the angle of gyration was set at 1.25° . The gyrations are applied at a rate of 30 revolutions per minute. The procedures of the DEM simulation process is summarized as follows:

- Generate compaction cylinder and funnel;
- Calculating particle numbers of each particle size according to gradation curve;
- Randomly generate particles in specific space (Figure 1a);
- Packing of spheres under gravity force until it is stable;
- Generate compression plate and gyratory compact asphalt mixture by constant pressure (Figures 1b and 1c);
- Record the position of compression plate and spheres during compaction process;
- Calculate air void of the whole mixture or each layer.



(a) (b) (c)

Figure 1: DEM Simulation Process

4 PACKING SIMULATION OF SINGLE-SIZED SPHERES

In order to validate the effectiveness of using DEM to simulate asphalt mixture compaction, random packing of single-sized spheres was first simulated with YADE. Random packing of spheres is a traditional and important problem that is very useful for many applications in physics, chemistry computer science, mathematics and engineering areas. It has attracted great interest and has been studied for many years since 1611 when Kepler first stated his famous conjecture about spheres packing (Scott 1960, Rutgers 1962, Matheson 1974, Aparicio and Cocks 1995).

For random packing there appears to be as yet no satisfactory theoretical approach and experimental analysis were mostly used in the past. In this study, a 3D DEM simulation was conducted to investigate random packing density of equal spheres. The rationality or irrationality of the results also can verify the correctness of using YADE to simulate particles packing. Five different sizes of spheres (4.75-, 9.5-, 12.5-, 19-, and 25-mm diameter) were randomly generated in space and elastic constitutive contact law was used.

According to Kepler conjecture, the highest possible density of equal-sized spheres is 74%. However, due to the effect of interaction and interference between spheres, it is impossible to achieve ideal packing situation and the real maximum density of equal-sized spheres is much lower than this value. Scott used 1/8 in. steel balls to study random packing and found a range of densities between 0.60 ~0.637 (Scott 1960). Rutgers obtained a similar range of densities with nylon balls (Rutgers 1962). In addition, researches also showed that the peripheral error due to the finite size of the containers should be taken into account. Scott and Aparicio both used linear regression curve to determine the average density for given size of containers to consider peripheral error (Scott 1960, Aparicio and Cocks 1995).

Figure 2 is the calculated results of packing density with respect to the relative scale (the ratio of sphere diameter to container diameter, d/D). The density curve shown in figure 2 presents the packing density increase with the decrease of relative scale (d/D) and the maximum packing density for equal size sphere is around 0.623, which was very close to the experimental results from other researchers' work. This implied that DEM code modified from YADE is effective in simulating random packing and can be used to investigate the compaction process of asphalt mixtures.

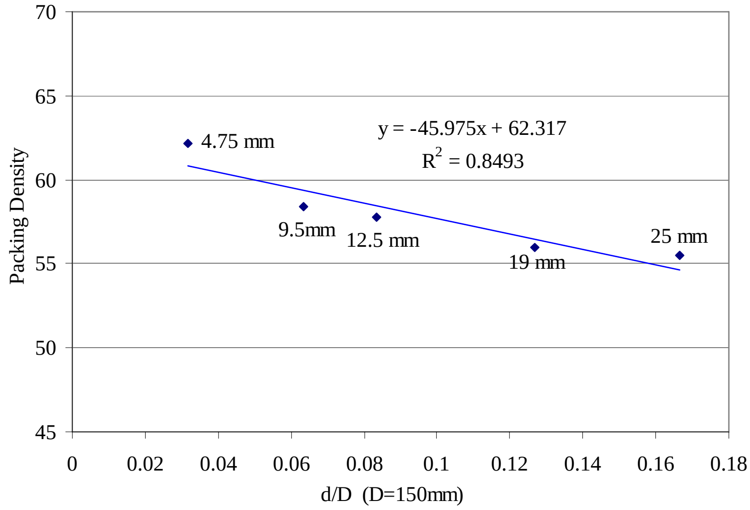


Figure 2: Packing Density with Respect to Relative Scale

5 SUPERPAVE GYRATION COMPACTION SIMULATION

5.1 Determination of Input Parameters

The overall constitutive behavior of a material is simulated by associating a simple constitutive model with each contact in discrete element method. Therefore, the contact behavior is an extremely important aspect in DEM, which may significantly influence the correctness and rationality of the model. Asphalt mixture is a thermal rheological material and its viscoelastic property should be considered during DEM numerical simulation. In this paper, in order to simulate the viscoelastic property of asphalt mixture, Burger's constitutive model was employed and a new constitutive law engine was developed in the YADE code to process the calculation.

To determine the input parameters of asphalt mixture, the common method is to obtain contact model's parameter by making regression analysis of experimental data. These laboratory tests usually include uniaxial creep test, stress relaxation test, and dynamic modulus test. Among these tests, dynamic modulus is a commonly used experiment to determine burger's parameters (Liu 2009, Abbas 2004) and therefore, was chosen in this paper. Since asphalt binder and fine aggregate (smaller than 2.36mm) ware assumed to mix together to form a special mastic, asphalt mastic samples (100mm in diameter and 150mm in high) were made for dynamic modulus test (Figure 3). The test device is produced by the IPC Global and the NCHRP 9-29 default values were used keep the strain between 75 and 125 micro-strain. The test was conducted at three temperatures (5°c, 20°c, 30°c) and ten frequencies (0.01, 0.1, 0.2, 0.5, 1, 2.5, 10, 20, 25 Hz) were selected. After testing, dynamic modulus master curves were constructed by translating the dynamic modulus curves at different temperatures to reference temperature. Usually, the master curve can be mathematically modeled by using a sigmoidal function and the master curve at any temperature can be obtained by applying Time-temperature superposition principle. The parameters of Burger's model can be calculated from dynamic modulus master curve by making nonlinear regression analysis. The specific regression procedure and function can be found in Abbas's research (2004). A regression program was compiled to do nonlinear regression analysis and the regression Burger's parameters are shown in table 1.

Figure 3: dynamic modulus test of asphalt mastic

Table 1: Burger's Model Parameters (at 150°C)

Parameters	E_1 (MPa)	η_1 (MPa·s)	E_2 (MPa)	η_2 (MPa·s)
Upper limit	23.086	1466.088	26.129	5.705
Mid value	21.025	1170.580	22.261	4.622
Low limit	18.650	810.537	15.789	2.235
Superpave	19.960	1030.856	19.255	3.717
SMA	15.996	652.714	10.891	1.898

5.2 SGC Simulation and Air Voids Estimation

Aggregate gradation for HMA has been studied by many researchers for a long time, but it still lacks an easy and effective theoretical method to establish a suitable gradation curve in mix design. In order to help engineers to determine reasonable aggregate gradation, some material standards give gradation limits as reference values, such as ASTM D3515. In this study, five types of aggregate gradation curves (upper limit, lower limit, mid value of ASTM gradation band, SMA aggregate gradation curve, and a Superpave aggregate gradation curve) were selected to investigate the effect of aggregate gradation. The position of the gyratory plate was recorded during virtual simulations of the compaction process and then converted into compaction curves. The gradation curves are shown in Figure 4. The compaction curves and results are shown in Figure 5.

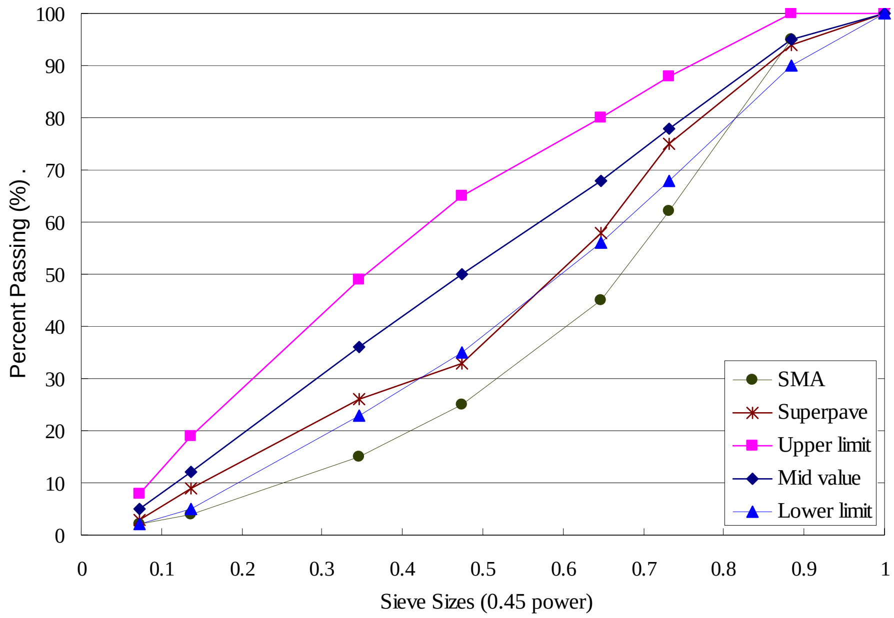


Figure 4: Aggregate Gradations

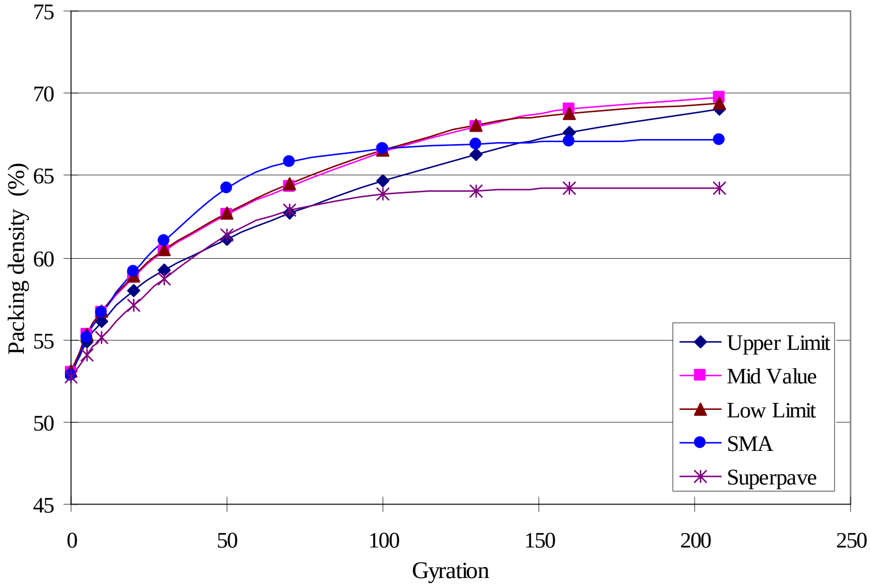


Figure 5: Compaction Curves (Aggregates bigger than 2.36mm)

Although aggregates smaller than 2.36mm were not considered in the present study, the air voids can be roughly establish according to the proportional relationship between compositions. It is assumed all fine aggregates and asphalt binder were filled into the voids between coarse aggregates, thus packing density is the proportion of coarse aggregates in the whole mixture. According to the proportional relationship between coarse and fine aggregates, the volume of fine aggregate in the whole mixture also can be calculated and the volume of asphalt can be calculated from the asphalt content in the whole mixture, thus the air voids can be roughly estimated (table 2).

Table 2: Air Voids Estimation

Proportion of composition (volume %)	Upper Limit	Mid Value	Low Limit	SMA	Superpave
Coarse aggregate (greater than 2.36 mm)	69.03	69.77	69.38	67.13	64.23
Fine aggregate (smaller than 2.36 mm)	66.41	39.25	20.84	16.78	22.57
Asphalt binder	18.70	15.00	12.39	11.58	11.96
“Air voids”	-54.13	-24.02	-2.61	4.52	1.24

As shown in Table 2, the “air voids” in the first three mixtures are negative values, which mean the coarse aggregate packing density is too dense to provide enough space for fine aggregates and asphalt binder. The extra fine aggregate and asphalt binder would segregate coarse aggregates and block the form of stone on stone contacts between coarse aggregates. Although the coarse aggregate packing density value of SMA and Superpave were lower than the first three aggregate gradations, the coarse aggregates can interlock with each other to form stable coarse aggregate structure and also provide sufficient voids for fine aggregates and asphalt binder which help bond the coarse aggregates together. Therefore SMA and

Superpave mixtures can also obtain pretty good performance behaviors, especially in high temperature rutting resistance.

During the compaction process, the geometrical information of spheres was recorded in specific gyrations and then used to calculate packing density. The specimen was divided into 44 layers to study the change of packing density in different gyrations. As shown in Figure 6, packing density of each layer generally increased with the increase in gyration number and the packing density was not uniform along the height of the specimen, which means the air voids distribution was not uniform along the specimen height. The shape of curves indicates that the top of specimen was compacted first and then the bottom of specimen. Finally the whole specimen was compacted and the compaction process was finished.

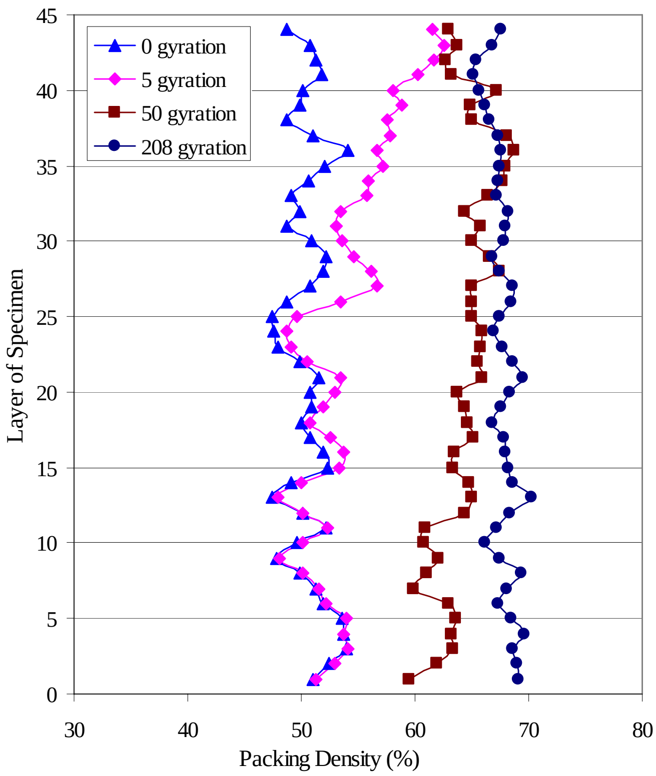


Figure 6: Packing Densities along Specimen Layers

6 SUMMARY AND CONCLUSION

A 3D DEM simulation has been carried out to study the compaction process of Superpave gyration compactor by using an Open Source discrete element code, YADE. Based on the simulation results, the following conclusions can be summarized:

- Due to the inherent advantages in granular materials analysis, DEM was an effective tool to simulate asphalt mixture compaction process and was potentially very helpful for selecting good aggregate grading for asphalt mix design by reducing the number of physical compaction in the laboratory.
- The packing simulation of single-sized spheres demonstrates that boundary condition had an impact on packing density. The maximum packing density for single-sized spheres was approximately 0.623, which agreed with the findings from literature.

- Aggregates gradation is an important factor affecting coarse aggregate packing density. Although the coarse aggregate packing density value of SMA and Superpave were lower than other three aggregate gradations, SMA and Superpave mixtures can still obtain pretty good performance behaviors by forming stable coarse aggregate structure.
- During the compaction process, the pressure first compacted the top of specimen and then to the bottom of specimen. Finally, the whole specimen was compacted.
- The SGC simulation results presented in this paper only consider the aggregates bigger than 2.36 mm and the aggregates were assumed to be spheres covered with asphalt mastic film. The account of fine aggregate in the simulation will significantly increase particle number and the DEM simulation can be simulated by using more powerful computer.

REFERENCES

Abbas, A. et al., 2007. *Micromechanical modeling of the viscoelastic behavior of asphalt mixtures using the discrete-element method.* International Journal of Geomechanics, vol. 7, n. 2, p 131-139

Abbas, A., 2004. *Simulation of the micromechanical behavior of asphalt mixtures using the discrete element method.* PhD Dissertation of Washington State University

Adhikari, S; You, Z; and Kutay, M.E., 2008. *Prediction of dynamic modulus of asphalt concrete using two-dimensional and three-dimensional discrete element modeling approach.* Geotechnical Special Publication, n. 179, p. 1020-1027

Birgisson, B., and Ruth, B. E., 2001. *Development of tentative guidelines for the selection of aggregate gradations for hot-mix asphalt.* ASTM STP 1412, ASTM, West Conshohocken, Page 110–127.

Chen, F., Eric, C.D. and Guiochon, G., 2007. *Prediction/Verification of Particle Motion in One Dimension with the Discrete-Element Method.* International Journal of Geomechanics, ASCE, Volume 7, Issue 5, pp. 344-352

Cundall, P. A., 1971. *A computer model for simulating progressive large scale movements in blocky rock systems.* Symposium of the International Society for Rock Mechanics, France, II-8

Huang, B. et al., 2009. *Effects of coarse aggregate angularity and asphalt binder on laboratory measured permanent deformation properties of HMA.* International Journal of Pavement Engineering Vol. 10, No. 1, Page 19–28

Jing, L., 2000. *Block system construction for three-dimensional discrete element models of fractured rocks.* International Journal of Rock Mechanics and Mining Sciences, Volume 37, Issue 4, Pages 645-659

John M. Ting et al., 1989. *Discrete Numerical Model for Soil Mechanics.* Journal of Geotechnical Engineering. Vol. 115, No. 3, pp. 379-398

Kim, H. and Buttlar, W.G., 2005. *Micro mechanical fracture modeling of asphalt mixture using the discrete element method.* Geotechnical Special Publication, n 130-142, pp. 209-223

Kozickij. and Donzef. V., 2008. *A new open-source software developed for numerical simulations using discrete modeling methods.* Computer methods in applied mechanics and engineering, vol. 197, pp. 4429-4443.

Liu, Y., Dai, Q., You, Z., 2009. *Viscoelastic Model for Discrete Element Simulation of Asphalt Mixtures.* Journal of Engineering Mechanics, Pages 324-333

Matheson, A.J., 1974. *Computation of random packing of hard spheres.* Journal of Physics C 7, pp. 2569-2576

Meegoda, J.N. and Chang, K.G., 1993. *Novel approach to develop a performance based test for rutting of asphalt concrete.* Pavement Innovations Theory to Practice, pp 126-140

Meegoda, J.N. and Chang, K.G., 1994. *Modeling viscoelastic behavior of Hot Mix Asphalt (HMA) using discrete element methods.* Proceedings of the Materials Engineering Conference, n 804, p 804-811

Aparicio, N. D. and Cocks, A.C.F., 1995. *On the representation of random packings of spheres for sintering simulations.* Acta Metallurgica et Materialia, Volume 43, Issue 10, Pages 3873-3884

Pan, T., Tutumluer, E. and Carpenter, S.H., 2005. *Effect of Coarse Aggregate Morphologyon the Resilient Modulus of Hot-Mix Asphalt.* Transportation Research Record: Journal of the Transportation Research Board, No. 1929, pp. 1–9

Roberts, F. L., Kandhal, P. S., Brown, E. R., Lee, D. Y., and Kennedy, T. W., 1996. *Hot mix asphalt materials, mixture design, and construction, 2nd Ed.*, NAPA Education Foundation, Lanham, Md.

Roque, R., S. Huang, and B. E. Ruth., 1997. *Maximizing shear resistance of asphalt mixtures by proper selection of aggregate gradation.* 8th Int. Soc. for Asphalt Pavements, Seattle, pp. 249–268

Rutgers, R., 1962. *Packing of Spheres.* Nature, Volume 193, Issue 4814, pp. 465-466

Scott, G. D., 1960. *Packing of equal spheres.* Nature, 188:908-909.

Vavrik, W. R., Huber, G., Pine, W. J., Carpenter, S. H., and Bailey, R., 2002. *Bailey Method for Gradation Selection in HMA Mixture Design.* Transp. Res. Circ., E-C044

Vavrik, W. R., W. J. Pine, G. A. Huber, S. H. Carpenter, and R. Bailey., 2001. *The Bailey Method of Gradation Evaluation: The Influence of Aggregate Gradation and Packing Characteristics on Voids in the Mineral Aggregate.* Journal of the Association of Asphalt Paving Technologists, Vol. 70, pp. 132–175

Wang, L.B. et al., 2007. *Fundamental mechanics of asphalt compaction through FEM and DEM modeling.* Geotechnical Special Publication, n 176, pp. 45-63, Analysis of Asphalt Pavement Materials and Systems: Emerging Methods

Xie, Y.S. and Zhao, Y.S., 2009. *Numerical simulation of the top coal caving process using the discrete element method.* International Journal of Rock Mechanics and Mining Sciences, v46, n6, pp. 983-991

You, Z. and Buttlar, W.G., 2004. *Discrete element modeling to predict the modulus of asphalt concrete mixtures.* Journal of Materials in Civil Engineering, v. 16, n. 2, pp. 140-146