DEM Approach for Engineering Aggregate Gradation and Shape Properties Influencing Mechanical Behavior of Unbound Aggregate Materials

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ABSTRACT: It has been well established that the mechanical behavior of unbound aggregate materials is strongly influenced by the shape of the particles and the complete grain size distribution (i.e., gradation). This paper presents the use of an image-aided discrete element method (DEM) approach to realistically model the micromechanical interactions of aggregate particles including size and shape effects. A realistic unbound aggregate model is developed from previous studies to simulate triaxial compression tests based on the DEM approach and the innovative use of membrane elements surrounding the cylindrical aggregate specimen in the DEM model. To calibrate the DEM model, six different types of aggregates were used to prepare samples of twenty-one unbound aggregate blends at the same gradation and voids content but different crushed percentages. The shape properties of flatness and elongation, surface texture and angularity were quantified by imaging then correlated to strength and permanent deformation characteristics obtained from triaxial testing. The experimental test results are utilized to determine required parameters for the discrete element model by minimizing the differences between DEM-simulated triaxial shear strength results and experimental ones. It is found that the developed DEM model is not only capable of reproducing the typical shear strength behavior of different unbound aggregate materials with varying shape properties, but also has the potential for optimizing the selection of size and shape properties of various unbound aggregates to achieve desired shear strength (or rutting resistance) and hydraulic behavior for open-graded permeable aggregate base.
INTRODUCTION

Unbound aggregate materials used in pavement foundation layer applications inherently consist of discrete grains that have varying shapes and sizes; therefore, they represent a granular assembly and modeling it as a continuum is not sufficiently correct. Furthermore, unbound aggregate particles transfer wheel loads through particle contacts forming the skeleton of aggregate structure, which contributes to the mechanical behavior and overall layer performance. To optimize the internal aggregate structure for improved resilient modulus \( (M_R) \), shear strength, and permanent deformation resistance, aggregate properties need to be properly selected.

In the past few decades, significant efforts have been made to better understand individual aggregate properties as factors influencing mechanical and hydraulic response trends of unbound aggregate materials \((1-5)\). The NCHRP Synthesis 382 reports the moisture content, dry density, soil classification, plasticity index (PI), percentage of materials passing No. 200 (or 0.075-mm) sieve (i.e., percent fines), and unconfined compressive strength among the most frequently used properties to correlate with \( M_R \) \((6)\). The impact of aggregate particle shape on the \( M_R \) and shear strength of pavement base/subbase layers has also been studied with the aid of imaging technology that quantifies aggregate morphology objectively and accurately. With the help of the University of Illinois Aggregate Image Analyzer (UIAIA), imaging-based particle shape indices (flat and elongation ratio, angularity, and surface texture) have been developed and successfully linked to the \( M_R \), strength and stability of aggregates \((7,8)\). Robust linkages between quantitative gradation characterization parameters and critical mechanical behavior of unbound aggregate materials were also explored for developing performance-based material specifications \((9,10)\).

Investigating material property effects through experimental methods requires a comprehensive, time-consuming, and labor-extensive set of experiments, yet still may not provide essential insight for understanding the underlying mechanisms. With the advent of computer technology, the discrete element method (DEM) pioneered by Cundall and Strack \((11)\) has been explored extensively as a powerful tool to model granular media. The most advantageous advantage of such a discrete-based DEM approach lies in the explicit simulation of particle movement (rotation, sliding, rearrangement, and crushing) under external loads by incorporating microscopic characteristics. In recent years, a variety of DEM simulations with different particles ranging from circular disk or spheres to tetrahedral or polyhedral particles have been attempted, along with the deformable DEM or combined finite/discrete element method \((12-14)\). Hill et al. \((15)\) presented a framework for a unified approach for modeling several laboratory tests used for the characterization of unbound materials for pavement applications, including the California bearing ratio (CBR) test, the dynamic cone penetrometer (DCP) test, and the \( M_R \) test. Although some limitations still exist, this proposed methodology is shown to be promising for developing mechanistic-based correlation between test results. Evans et al. \((16)\) simulated biaxial compression tests on two-dimensional (2D) particulate assemblies for four gradation curves and interpreted material responses in terms of stress-strain-strength behavior at the macro scale and particle-level properties at the micro scale. Tutumluer et al. \((17)\) evaluated different AREMA gradations currently in use for their effects on both...
ballast void space and load carrying performances using the University of Illinois ballast DEM model BLOKS3D program. In summary, the DEM approach has been demonstrated as quite promising in identifying differences in base/ballast material specifications in terms of structural support and drainage as well as providing new insight into optimizing unbound aggregate gradations for better performance.

One major obstacle that hinders the widespread applications of the DEM approach to pavement unbound aggregate materials is, however, the unaffordable simulation time required, which is the function of both sample size (a function of the maximum particle size) and the minimum particle size. The size of the particles used in a DEM simulation determines both the number of particles and the time step. Actual gradation curves of pavement base/subbase materials are typically widely-ranged with a minimum particle size of around 0.075 mm and a maximum one of up to 50 mm. The unreasonably high number of DEM particles and small time step required would demand massive computational resources and thus prohibit parametric studies with multiple simulations and configurations. As a compromise, the actual particle size bins were scaled up and/or mapped into narrower margins in previous studies to generate analogous grain size distributions to realistic ones so that a much more practical number of particles is yielded in DEM simulation (16,18).

OBJECTIVES AND SCOPE

The primary objective of this paper is to calibrate an image-aided DEM program BLOKS3D developed at the University of Illinois (19) against laboratory rapid shear strength (triaxial compression) test results and determine DEM model parameters. Once calibrated and validated, such a DEM program could be potentially utilized to investigate effects of multi-scale aggregate gradation and morphological properties on structural performances of unbound aggregate pavement layers. The relationships among the microscopic internal structure, micro-mechanical parameters, and macroscopic responses could also be identified from DEM based numerical simulations. Based on the DEM approach, the ultimate goal is to further engineer current base/subbase material specifications by optimizing the gradation and shape properties which minimizes the overall rutting potential (based on shear strength behavior) yet still accommodates desired drainage requirements.

DESCRIPTION OF LABORATORY RAPID SHEAR TESTS

The coarse aggregate materials used in the laboratory study consisted of the most commonly used crushed aggregate types in the paving industry, i.e., limestone, gravel, sandstone, granite, and slag. The six unblended aggregate samples are listed in Table 1, along with their relevant physical properties and rapid shear and permanent deformation test results. The angularity index (AI) and surface texture (ST) index of those aggregate samples were quantified from three orthogonally acquired two-dimensional (2D) images of individual particles using the UIAIA (7,20). None of these coarse aggregate samples has flat and elongated particles exceeding 10% by weight of greater than 5 to 1 (>5:1) longest to shortest dimensions. To minimize the influences of maximum aggregate sizes and/or gradations, all the specimens were...
prepared according to the same gradation with the same top aggregate size of 38 mm (see Figure 1a). Additionally, each crushed aggregate type was blended with uncrushed gravel at 0, 50, 67, 83, and 100% by volume fractions to generate a total of 21 aggregate blends for studying the effect of blending two different types of aggregates on the strength and rutting behavior, respectively (8). Figure 1b illustrates that the blending with different crushed materials improved both shear strength and rutting resistance behavior of the uncrushed gravel. This is due to the fact that blending in this case results in more desirable aggregate shape properties than the uncrushed gravel.

The 21 aggregate blends were tested in dry (0% moisture content) condition with no fines included in gradation. Each specimen was prepared 152 mm in diameter and 305 mm in height. The same void ratio of 67.5% (or porosity of 41%) was achieved for all triaxial rapid shear aggregate specimens by controlling the total volume of the aggregate particles contained in the specimen. The rapid shear test performed is a deformation controlled test with an axial strain of 12.5% (corresponding to 38 mm) obtained in 1 second at the confining pressure of 34.5 kPa. Such a loading rate is reported to be highly effective in characterizing the bearing capacity failure of the unbound aggregate base/subbase layer under moving traffic loading (2). In this study, the maximum deviator stress at failure \( \sigma_d \) measured from only one rapid shear test at 34.5-kPa confining pressure is used as an indicator of the shear strength of each aggregate blend (see Table 1), instead of the friction angle and the cohesion intercept.

DISCRETE ELEMENT MODELING OF RAPID SHEAR TESTS

Particle Sizes and Shapes

The actual gradation (see Figure 1a) has a minimum aggregate size of 6.3 mm and a maximum aggregate size of 38 mm, which requires approximately 1,800 polyhedral particles in the DEM simulation with a time step of around \( 2.73 \times 10^{-7} \) s, given the specified specimen dimensions. A set of particle shapes was selected from the pre-established DEM particle shape library to match the measured shape indices for each aggregate blend (see Table 1), respectively. More details about the DEM particle shape library can be found elsewhere (13). During particle generation, particle geometries were randomly chosen from the selected set of particle shapes.

Simulation of a Flexible Membrane and Rigid Platens

To model flexible membrane, the approach documented by Lee et al. (18) was used. Specifically, a total of 240 rigid rectangular cuboid discrete elements are positioned in a cylindrical arrangement to form a hollow space of 152.4-mm (6-in.) inner diameter and 304.8-mm (12-in.) height, respectively. The particles are positioned inside the hollow cylinder. As shown in Figure 2a, the height of the cylinder is divided into 10 layers each of which is 30.48 mm high, and the circumference of each layer is simulated with 24 membrane elements. Each membrane element has a thickness of 4 cm and a surface area of 10 cm by 5 cm, which allows some initial overlap between
neighboring membrane elements. To mimic the specimen deformation in the experiments, each membrane element is only allowed to have translation movement in radial direction and is independent of that of neighboring ones, with all the other degrees of freedom restricted. The external radial concentrated force is applied at the center of each membrane element and continuously adjusted to result in a constant confining cell pressure. The top platen is simulated as a frictional rigid rectangular cuboid element with a thickness of 2 cm and a square cross sectional area of 30 cm by 30 cm. The shearing of the aggregate specimen is controlled through vertical displacement of the frictional rigid platen. No contact detection is performed between any two membrane elements or between platens and membrane elements. The friction angle between aggregate particles and membrane elements is set to zero throughout the simulations. The material properties of the platen are approximated to be the same as those of the aggregate particles.

**Sample Preparation and Shearing Procedure**

While detailed descriptions can be found elsewhere (14,18), the sample preparation process is illustrated in Figure 2 and briefly presented as follows: (i) generation of membrane elements and the top platen according to specified arrangement; (ii) particle generation with a target initial void ratio according to the prescribed gradation (different void ratios are achieved by changing either inter-particle friction angles or the gravitational acceleration); and (iii) simultaneous application of (isotropic) confining pressure upon the top platen (in vertical/axial direction) and membrane elements (in radial direction). Once the sample preparation is complete, shearing of the aggregate specimen is performed by applying incremental vertical displacements on the top platen. Note that the particle-particle and platen-platen friction angles and the gravity constant are re-set to their desired values prior to shearing.

In the laboratory rapid shear test, the sample was sheared at a rate of 31 mm (1.25 in.) per second. To avoid a long run-time as well as computational stability problem caused by dynamic effect during continuous shearing, the incremental shearing scheme reported elsewhere is adopted herein to reproduce the shearing process (14,18). Note that rapid shear tests performed on railroad ballast materials were found not sensitive to strain rate and thus can be treated as a quasi-static problem according to Qian et al. (14). The top platen is moved discretely by 0.01 mm (0.01% of axial strain) in each increment. Immediately after each incremental displacement, the platen is fixed in its new position and the simulation is continued to allow the particles and the membrane elements to re-equilibrate under this new boundary condition until the changes of both vertical and horizontal effective stresses are below a desired tolerance level. Once equilibrium is reached, vertical and horizontal effective stresses and volumetric strain are recorded. In this study, all simulations were carried up to 7% axial strain based on laboratory experiment results.
FIG. 1. Gradation curve of aggregate specimens (a) and aggregate blending effect on maximum deviator stress $\sigma_d$ (b) and permanent strain $\varepsilon_p$ (c).

Table 1. Aggregate Types and Test Results

<table>
<thead>
<tr>
<th>Aggregate Types *</th>
<th>Angularity Index (AI)</th>
<th>Surface Texture Index (ST)</th>
<th>Specific Gravity ($G_s$)</th>
<th>Specimen Weight (grams)</th>
<th>Max. Deviator stress $\sigma_d$ at Failure (kPa) **</th>
<th>Plastic strain $\varepsilon_p$ at N=10,000 (%) ***</th>
</tr>
</thead>
<tbody>
<tr>
<td>Uncrushed Gravel</td>
<td>252</td>
<td>0.9</td>
<td>2.583</td>
<td>8535</td>
<td>270.2</td>
<td>1.81</td>
</tr>
<tr>
<td>Crushed Granite</td>
<td>550</td>
<td>2.4</td>
<td>2.622</td>
<td>8664</td>
<td>710.2</td>
<td>0.61</td>
</tr>
<tr>
<td>Crushed Limestone</td>
<td>495</td>
<td>1.75</td>
<td>2.735</td>
<td>9037</td>
<td>510.2</td>
<td>1.15</td>
</tr>
<tr>
<td>Crushed Gravel</td>
<td>371</td>
<td>1.09</td>
<td>2.548</td>
<td>8419</td>
<td>420.6</td>
<td>1.35</td>
</tr>
<tr>
<td>Slag</td>
<td>516</td>
<td>2.2</td>
<td>2.435</td>
<td>8046</td>
<td>531.0</td>
<td>0.87</td>
</tr>
<tr>
<td>Sandstone</td>
<td>402</td>
<td>1.82</td>
<td>2.270</td>
<td>7501</td>
<td>482.6</td>
<td>1.07</td>
</tr>
</tbody>
</table>

*Void ratio=67.5% (porosity=41%); **Confining pressure $\sigma_3$=34.5 kPa; ***$\sigma_3$=34.5 kPa, bulk stress $\theta$=172.4 kPa.
FIG. 2. Illustration of triaxial compression DEM simulation: (a) arrangement of membrane elements, (b) aggregate specimen modeled, and (c) specimen preparation process.

CALIBRATION OF THE DEM MODEL WITH RAPID SHEAR TESTS

The purpose of the calibration process is to select appropriate micro-parameters required in DEM simulations. Among required modeling parameters in the DEM simulation, particle shape and size are already chosen according to prescribed gradation, while inter-particle friction angle ($\phi'$), normal contact stiffness ($K_n$), shear contact stiffness ($K_s$), and contact damping ratios remain to be selected. The global damping ratio is neglected in this study. Those micro-mechanical parameters, which generally do not represent real mechanical properties and are difficult to obtain experimentally, are found by a trial and error procedure such that the simulation yields similar macroscopic (global) behavior as that of the aforementioned laboratory rapid shear tests. As compared to the normal and shear contact stiffness values, the inter-particle friction angle is reported to have a greater influence on the simulation results (18). To be specific, the normal and shear contact stiffness values are first kept constant; while the inter-particle friction angle that mainly depends on the particle surface roughness (i.e., the particle mineralogy) is varied within the typical range reported previously (21). After selecting a proper inter-particle friction angle that results in simulated responses comparable to experimental data, the normal and shear
contact stiffness values are then varied for calibration. For numerical stability, the shear contact stiffness value is chosen to be smaller than the normal contact stiffness value. For the very first trial, the stiffness values (K_n=20 MN/m and K_s=10 MN/m), successfully employed in prior studies (13,14) to simulate granite ballast behavior, were used. This procedure was repeated until final stiffness values were selected. Since the critical time step for numerical stability is inversely proportional to the normal contact stiffness, the smallest normal contact stiffness value that matches experimental results fairly well was selected to allow for a larger simulation time step. It is worth noting that multiple simulations with different initial conditions (as resulted from randomly selecting DEM particle assembly from the pre-chosen particle library) were not performed in this study.

After a series of trials, the final parameters determined for the DEM simulation are listed in Table 2. The particle elastic modulus and Poisson’s ratio are fixed at 97.9 MPa and 0.25, respectively. The contact damping ratio is set as 0.03. The DEM simulation results obtained using calibrated micro-mechanical parameters are tabulated in Table 3 where satisfactory agreement is achieved. The DEM-predicted deviator stresses match closely with those from experiments, which means that the developed DEM model is capable of reproducing the typical mechanical behavior of unbound aggregate materials. The DEM simulations were carried out past each peak value of the deviator stress. Figure 3 shows the numerical results obtained with the micro-parameters reported in Table 2 at 34.5-kPa confining pressure level for uncrushed gravel, slag, and crushed granite specimens, as these three specimens represent three distinguishing deviator stress levels (i.e., high, medium, and low). It was revealed from DEM simulation results that the nonlinear stress-strain behavior of unbound aggregate materials (including dilatancy effects) was properly simulated by the DEM model.

According to the linear Mohr-Coulomb model, which is typically used to represent the shear strength of granular materials, the relationship between shear stress at failure (τ_f) and normal stress (σ_n) is described as a function of the cohesion (c) and angle of internal friction (φ), i.e., τ_f = c + σ_n tan φ. Despite the argument by many researchers whether c represents the material’s “true” cohesion or merely a parameter of a linear fit of the linear Mohr-Coulomb model, c is assumed to be zero for aggregate specimens in this study which were sheared under dry conditions. As a result, the peak principal stress ratio (PSR) for a linear Mohr-Coulomb model is calculated for each DEM simulation to compute the peak friction angle (φ_P) as:

\[
φ_P = \sin^{-1}\left(\frac{σ_1/σ_3 - 1}{σ_1/σ_3 + 1}\right)
\]

where φ_P is peak friction angle; and σ_1 and σ_3 are major and minor principal stresses, respectively. Figure 4 shows the variation of φ_P with aggregate shape indices. Note that the peak friction angle φ_P increases with increased angularity index (AI) and surface texture (ST) values, indicating improved shear resistance.
Table 2. Calibrated DEM Model Parameters

<table>
<thead>
<tr>
<th>Aggregate Types</th>
<th>Uncrushed Gravel</th>
<th>Crushed Granite</th>
<th>Crushed Limestone</th>
<th>Crushed Gravel</th>
<th>Slag</th>
<th>Sandstone</th>
</tr>
</thead>
<tbody>
<tr>
<td>Friction Coefficient $f (\tan \phi')$</td>
<td>0.42</td>
<td>0.75</td>
<td>0.6</td>
<td>0.52</td>
<td>0.65</td>
<td>0.6</td>
</tr>
<tr>
<td>Normal Contact Stiffness $K_n$ (MN/m)</td>
<td>10</td>
<td>40</td>
<td>20</td>
<td>20</td>
<td>20</td>
<td>20</td>
</tr>
<tr>
<td>Shear Contact Stiffness $K_s$ (MN/m)</td>
<td>5</td>
<td>20</td>
<td>10</td>
<td>10</td>
<td>10</td>
<td>10</td>
</tr>
</tbody>
</table>

Table 3. Triaxial Compression DEM Simulation Results

<table>
<thead>
<tr>
<th>Aggregate Types *</th>
<th>Void Ratio $e$ (%)</th>
<th>Specimen Weight (g)</th>
<th>Max. Deviator Stress $\sigma_d$ at Failure (kPa) *</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Lab DEM</td>
<td>Lab</td>
<td>Lab DEM</td>
</tr>
<tr>
<td>Uncrushed Gravel</td>
<td>67.5</td>
<td>8535</td>
<td>8535</td>
</tr>
<tr>
<td>Crushed Granite</td>
<td>66.9</td>
<td>8664</td>
<td>8693</td>
</tr>
<tr>
<td>Crushed Limestone</td>
<td>66.1</td>
<td>9037</td>
<td>9111</td>
</tr>
<tr>
<td></td>
<td>67.5</td>
<td>8535</td>
<td>8535</td>
</tr>
<tr>
<td>Crushed Gravel</td>
<td>67.0</td>
<td>8419</td>
<td>8442</td>
</tr>
<tr>
<td>Slag</td>
<td>67.8</td>
<td>8046</td>
<td>8030</td>
</tr>
<tr>
<td>Sandstone</td>
<td>66.3</td>
<td>7501</td>
<td>7554</td>
</tr>
</tbody>
</table>

* $\sigma_3=34.5$ kPa.

FIG. 3. Triaxial compression DEM test results for three specimens representing high, medium, and low maximum deviator stress levels.
FIG. 4. Variation of peak friction angle ($\phi_P$) with angularity index AI (a) and surface texture ST (b).

DEM APPROACH FOR OPTIMIZING PERMEABLE AGGREGATE BASE GRADATION

The DEM model calibrated for six different aggregates has the promising potential to be applied to engineer the gradations of permeable (open-graded) aggregate base (PAB) materials. Using an open-graded aggregate base has been demonstrated to be one of the effective strategies for improving drainage efficiency and thus pavement longevity. For example, in Minnesota, two main permeable base materials are widely used, i.e., stabilized and unbound. In addition to maintaining adequate permeability, these layers are also required to remain stable during construction as well as future rehabilitation activities over the design service life. An ongoing research study is focused on analyzing Minnesota DOT (MnDOT) aggregate gradation specifications for PAB materials (see Figure 5a) with the goal to recommend an optimal gradation that is not only qualified as drainable aggregate base but also potentially yields optimized strength and deformation characteristics. According to a “gravel-to-sand” ratio concept recently proposed by Xiao et al. (9) from the preliminary experimental studies for optimizing unbound aggregate gradations for improved shear strength behavior (Figure 5b), a drainable aggregate base was already recommended that needs to include a significant amount of recycled Portland cement concrete (PCC) to support a new PCC pavement on MnROAD test Facility 2013 Test Section 13 reconstruction (an interstate test section). Such a recommended material gradation is shown in Figure 5a along with current MnDOT PAB specifications. As a reference, another gradation (Ohio DOT C307-IA for drainable bases) with proven field performance (22) is also illustrated. Figure 5a indicates that these two drainable gradations are actually very close to each other, hence the promising application of the gravel-to-sand ratio concept for gradation optimization. Future efforts will be dedicated to verifying and optimizing the shear strength behavior of this gradation through the DEM triaxial compression test simulations with aggregate shape and size effects taken into account.
FIG. 5. (a) MnDOT gradation specifications for unbound and stabilized permeable aggregate bases (PAB); (b) gradation chart with contours of the gravel to sand (G/S) Ratio gradation parameter for MnDOT unbound PAB gradation band.

CONCLUSIONS

It has been well established that the mechanical behavior of unbound aggregate materials is strongly influenced by the shape of the particles and the complete grain size distribution (i.e., gradation). Six different types of aggregates were used to prepare samples of twenty-one unbound aggregate blends at the same gradation and voids content but different crushed percentages. The shape properties of flatness and elongation, surface texture and angularity were quantified first by imaging and then correlated to strength and permanent deformation characteristics obtained from triaxial testing. Aggregate blending for more desirable angular and rough surface textured aggregate shape properties, as compared to the original uncrushed gravel, improved both shear strength and rutting resistance behavior of the uncrushed gravel. The peak friction angle $\phi_P$ (with cohesion $c$ neglected due to dry specimens tested with no fines, i.e., 0% passing No. 200 sieve or 0.075 mm size) increased with increased angularity index (AI) and surface texture (ST) values.

To realistically model the micromechanical interactions of aggregate particles including size and shape effects, this paper introduced the use of an image-aided discrete element method (DEM) approach. Laboratory rapid shear (triaxial compression) tests were simulated based on the DEM approach and the innovative use of membrane elements surrounding the cylindrical aggregate specimen in the DEM model. The aforementioned experimental test results were utilized to determine required micro-mechanical parameters for the DEM model by minimizing the differences between the DEM-simulated triaxial shear strength results and experimental ones. It is confirmed from DEM test results that the nonlinear stress-strain behavior of unbound aggregate materials, including dilatancy effects, could be
properly simulated by the DEM approach. The predicted deviator stresses matched closely with those from the experiments, indicating the capability of the developed DEM model to reproduce the typical shear strength behavior of unbound aggregate materials. For future efforts, the calibrated DEM model has the potential for optimizing the selection of size and shape properties of various types of unbound aggregates to achieve desired shear strength (or rutting resistance) and hydraulic conductivity or drainage characteristics (function of aggregate shape and air void distribution) for open-graded permeable aggregate base.

ACKNOWLEDGMENTS

The work reported in this paper was completed as part of an ongoing Minnesota DOT research study (Contract #89260), entitled, "Cost Effective Base Type and Thickness for Long Life Concrete Pavements." The authors acknowledge MnDOT Office of Materials and Road Research for the support. Special thanks are due to Mr. Terry Beaudry (MnDOT), Chair of the Technical Advisory Panel, Dr. W. James Wilde (Minnesota State University, Mankato), the Co-PI, Mr. John Siekmeier (MnDOT), and Mr. Mark Watson (MnDOT) for providing technical guidance and coordination. The authors also acknowledge Professors Youssef Hashash and Jamshid Ghaboussi and Mr. Seung-Jae Lee involved with the Discrete Element Method modeling research activities at the University of Illinois. The contents of this paper do not reflect the official views or policies of MnDOT. This paper does not constitute a standard, specification, or regulation.

REFERENCES


