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UTILIZING A PARTICLE FLOW CODE IN 2 DIMENSIONAL DISCRETE ELEMENT METHOD OF FRACTURE RESISTANCE EVALUATION OF HMA AND BRITTLE ROCK

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ABSTRACT

Recently researchers and engineers have been in favour of optimized and efficient designs of all different types of structures, by directing their attention to non-destructive testing and most importantly computer simulations. Thus avoiding time consuming testing, and understanding the true behavior of materials within structures under different loading setups. One of the newly used computer aided analysis methods employed today is the discrete element method (DEM) embedded in PFC computer software. The main purpose of the DEM modeling conducted for this study was to supplement previous research conducted into the area of hot mix asphalt and rock fracture evaluation. The models created for this study demonstrated that PFC software is a powerful analysis tool that can be adapted to a variety of scientific and engineering applications, and has proved to be a very useful tool for modeling several HMA laboratory tests, and with proper modification it can also be adapted to modeling many other materials.

Keywords: Numerical modeling; discrete element method; fracture evaluation; hot mix asphalt; brittle rocks.

1. INTRODUCTION

One of the most popular themes in today's engineering world is optimized and efficient design of all different types of structures, machines, tools and other man made devices. As our scientific understanding of the materials used in these applications and the associated mathematics has improved so has the desire to make them perform at a higher level and

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more economically. To assist engineers and other scientists in the evaluation of these products, many different tools have been developed. One of the most common computer aided analysis methods employed today is finite element analysis (FEA). The discrete element method (DEM) is similar to FEA, but incorporates several additional parameters that make it ideally suited to a wide range of applications including areas such as granular flow and rock mechanics.

The main purpose of the DEM modeling conducted for this study was to supplement previous research conducted into the area of hot mix asphalt and rock fracture evaluation. To expedite the Hot Mix Asphalt (HMA) and rock fracture analysis, it was proposed to develop a DEM model that could accurately predict the expected failure pattern and corresponding stresses. The goals of developing the model were to verify the laboratory testing results, observe the crack propagation pattern though a specimen, create an alternate, nondestructive fracture prediction method, and to aid in future laboratory testing of HMA samples. In addition to HMA testing model, another model was created in association with the shear failure testing setup for brittle rock. The results of this model will also be discussed in this paper.

2. BACKGROUND

Discrete element method (DEM) models the movement and interaction of circular particles, as described by Cundall and Strack [2]. The original implementation of this method was as a tool to perform research into the behavior of granular materials [1-11]. It is now utilized in different research arenas, such as medical and biomechanics [12,13], petrochemical engineering [14], fluid mechanics [15], and structural engineering applications [16-20]. The particles model was used successfully to simulate element behavior in real problems that involve complicated deformation patterns [22].

The need for the DEM models arose from an existing study investigating the fracture evaluation of HMA samples for use in the Superpave mix design method. Historically, the investigation the fracture resistance assessment of HMA specimens was conducted by means of the single edge notched beam (SENB) test [1]. This analysis used a rectangular notched beam tested in three-point loading to determine the mixes bending properties and fracture resistance. More recently the use of a semi-circular notched beam (SCNB) to evaluate HMA specimens has been adopted in many research studies [1]. Research has shown the SCNB test to be sensitive to asphalt mix properties and to accurately characterize the fracture resistance of asphalt mixes. The initial two DEM models were created to verify the results of the SCNB and SENB laboratory tests and the FEA model that was constructed as part of the existing study. The geometries for the SCNB and the SENB tests are shown below in Figure 1.

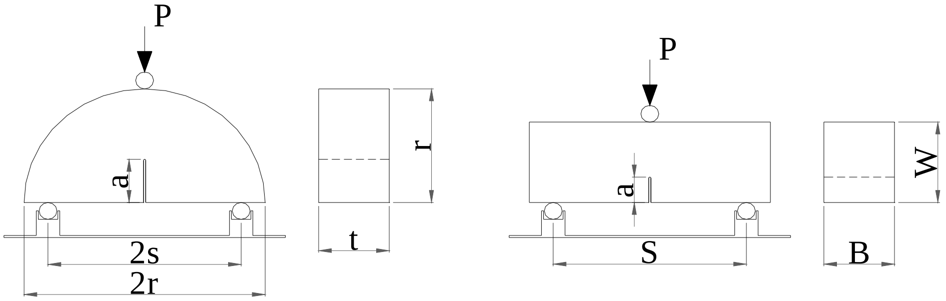

Figure 1. SCNB and SENB test geometries [1]

For this study the required models were developed using the Particle Flow Code in 2 Dimensions (PFC2D) software produced by Itasca [22]. This software models the interaction of circular particles using DEM. PFC2D software also accommodates the evaluation of noncircular particles by allowing the user to clump multiple circular particles together into the desired shapes. Although the software was initially developed for the evaluation of granular flow, it can be used to model brittle solids by bonding all adjacent particles to its neighbors and can fracture when the bonds are broken in a progressive pattern. The analysis of both homogeneous and non-homogeneous materials is possible in PFC2D by assigning different properties to different regions of the model.

Since PFC2D only supports circular elements, the largest drawback of using this software is that there can be no planar edges. No matter the arrangement of the circular particles there will always be irregular edges. This drawback is offset by the ease of detecting contacts between circular particles, which is a great deal more efficient than with angular elements. Also as stated above, with the PFC2D it is possible for the model to break, unlike FEA models or other available DEM software [22]. These advantages make DEM analysis via PFC2D software ideal for achieving the goals of this research.

In PFC2D the circular elements are referred to as balls and the supporting/confining lines and curves are called walls. The main properties for both of these objects are; normal and shear stiffness and friction coefficient. The balls must be assigned a density as well. Two bonding mechanisms are included in the PFC software, with the option for the user to create and use a different model if they desire. Contact bonds and parallel bonds are the original contact models included in the software. Contact bonds can be created between any elements that are in contact and have both normal and shear strength. These bonds do not resist moments and allow the particles to rotate about each other if additional bonds are not present. Parallel bonds are the second type of bond included in the software. The main difference between these bonds and contact bonds is that parallel bonds have a thickness bonds and can therefore resist moments. The properties of all of these objects (balls, walls and bonds) can be modified as the model is built or at any time during the analysis.

Once a model has been specified in PFC2D, a solution to a given set of conditions is found through an iterative time step process. For each time step Newton's Second Law is integrated twice for each particle in the model. The result of this calculation is a new velocity and position for each particle. Then based on the new position and velocity values, new contact forces and displacements are determined. New bond forces are also calculated at each time step and if the new force exceeds the user specified value for a specific bond, then that bond breaks and ceases to exist in the model allowing the two particles to move independently. Once a bond is broken the interaction between the adjacent particles is based on friction. The analysis process continues in the manner described above for the user specified number of time steps [22]. The process of creating a model to accurately represent actual materials is very involved and takes much more trial and error than is readily apparent from the basic modeling concepts presented above. More of the detail that went into attempting to create these models will be presented in the following sections as it relates to each model and the specific difficulties of the different materials that the model is attempting to closely approximate.

3. PFC MODELS

3.1 SCNB Model

The first model created related to the newer SCNB test for the evaluation of HMA samples. Before the first versions of the model were created it was necessary to become familiar with the use of PFC2D software. The user-guide provided with the software gives very detailed information about the different commands in the software and includes a number of well formed example problems to help new users become accustom to the method of command entry. In PFC2D, all of the commands are typed in or read by the software from existing text files. The majority of the commands require multiple inputs for the command to be executed correctly. So until the user has become quite familiar with the commonly used commands it is necessary to refer often to the command guide book.

Once a sufficient understanding of the software basics had been attained work began on the first model. The original model was intended to be made up of a wide range of particle (circle) sizes to approximate the irregular matrix of the cross-section of a HMA sample. During this initial phase of modeling the desired outcome was to create a model that would crack (fail) in a similar pattern to the physical samples tested in the lab. For the first version of this model no clumping was used, so all of the individual particles remained circular. Although this was not an extremely accurate method of representing an HMA cross-section, it was deemed reasonable for the preliminary designs. If possible, the accuracy of this model would be improved by using the clump logic in PFC2D to create irregularly shaped particles in later versions. Figure 2 below shows the cross-section a laboratory HMA specimen and the first version of the PFC model.

The model shown in Figure 2 was constructed by first specifying the outer edges of the model and then filling the interior with a wide range of element sizes selected by the user and placed randomly by the software. Once the elements were placed it was necessary to perform a "packing" procedure to create a dense mesh. If this is not done, then some of the elements may not be touching the adjacent elements and therefore would not become bonded together when the bonds are added.

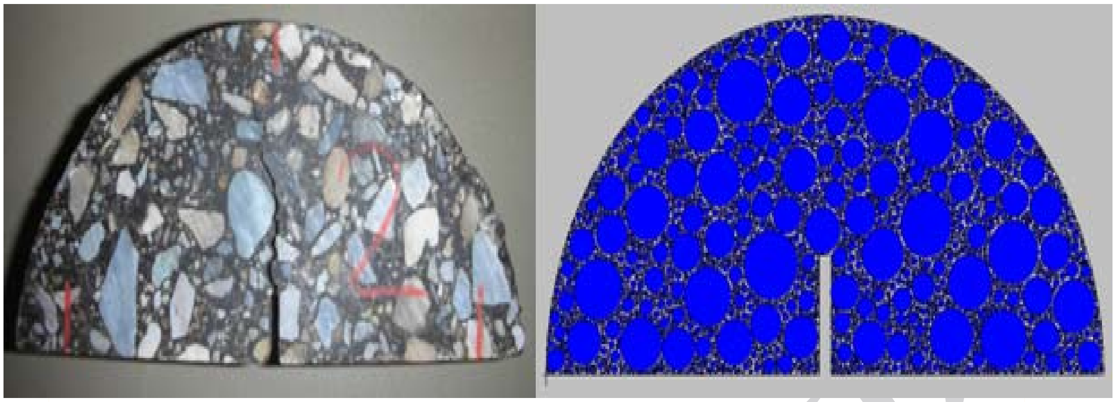

Figure 2. Laboratory HMA specimen and early version PFC model

In the PFC2D user guide [22] a process for creating a dense mesh is outlined, where the user increases the radius of each particle in the model by the same factor. This process should cause some of the particles to overlap, which results in contact forces. Then, by cycling (time stepping) the model can be brought to a state of equilibrium. When the model consists of a finite number of particles it is possible to do this quickly, but the model shown above in Figure 2 contains approximately 5000 particles and so cycling to equilibrium took a significant amount of time and cycles.

At this point one of the most difficult issues of working with PFC2D was encountered for the first time. Due to the freedoms associated with the DEM analysis in PFC2D software, the specification of material properties and analysis conditions can be quite complicated. In most engineering analyses the only properties that engineers are concerned with are the macro properties of the material, which in the case of HMA are the properties of the aggregates and the mastic (asphalt binder and fine aggregates) that can be measured in a lab. For the PFC2D analysis it is necessary to input the micro properties of the material, which for HMA relate to the contacts between particles in the model and bond strength values [23].

Without the correct macro properties from lab testing the micro properties for the PFC2D model cannot be calculated. For this specific study the necessary macro property values were not available so it was necessary to approximate values for the micro properties that would allow the model to function as desired. If lab testing had been conducted then it would have been possible to use the equations outlined by Yu et al. [23] to determine the correct micro properties for this analysis.

The initial trials for the first model consisted mainly of attempting to establish reasonable micro property values for the simulation. For this model the load was modeled as a separate ball particle and the base supports were modeled as semi-circular walls. The normal and shear stiffness for particles, bonds and supports were the parameters that were varied in these early trials. For simplicity contact bonds were used, since they require less property inputs.

Many of these attempts had unacceptable results. Often the bonds would be so weak that the load and support particles would easily shear through the cross-section breaking all of the bonds and leaving the elements scattered all over the screen. The opposite was also a common early result, where the bonds were far too strong and the applied loads had only a minimal effect on the model.

The best outcome obtained from this first set of models was achieved when the entire model held together and flexed under the load. As the load was applied the notch in the base of the model bowed outwards and grew to more than 4x the original length. Although there was a large amount of deformation the model continued to behave elastically and no crack developed. At this point a new approach was chosen that had results which were much more consistent with lab test results.

In the next version of the SCNB model a homogeneous set of elements arranged in rows was used, where as in the previous model particles of various sizes with random placement had been used. This model did not include clumped elements to represent the aggregates since the first goal was to develop a straightforward model that would accurately show the crack propagation through the model. Once this was achieved it would be possible to add clumped particles to represent the aggregates in the future.

One of the major benefits of using a homogeneous configuration was that it was not necessary to use the packing procedure described above which greatly decreased the amount of time needed to analyze the model. In order to bunch as many particles as possible in the model the rows were offset by the ball radius and stacked as shown below in Figure 3. Staggering the rows and bunching the balls together also helped to reduce the void space in the model.

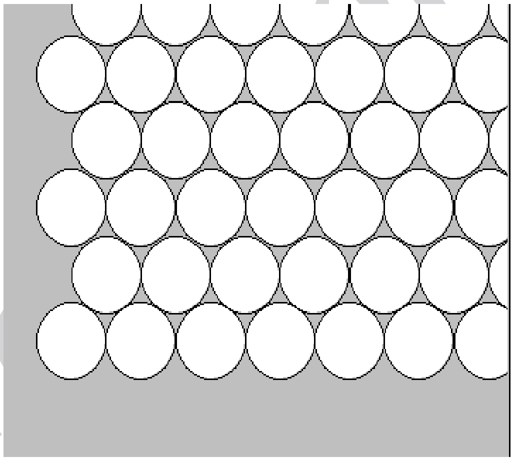

Figure 3. Element arrangement (SCNB model)

As with the previous model it was necessary to establish acceptable micro parameters for the model through trial and error. However, this time once the correct properties had been achieved the results were much more acceptable. The image on the left in Figure 4 below shows the completed homogeneous SCNB model and the growth of the crack. This crack propagation pattern compares quite well to the results of the laboratory testing which can be seen in Figure 2. To further verify the results of this model, the tensile stress at the tip of the notch was measured and compared to the values from FEA performed previously [1]. On the right side of Figure 4 is the graph of the tensile stress at the notch tip from the DEM model.

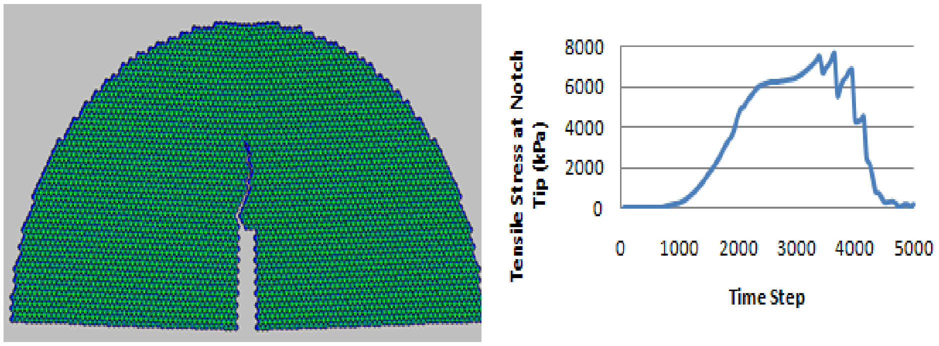

Figure 4. SCNB model with crack and plot of tensile stress at notch tip

3.2 SENB Model

Once acceptable results had been achieved for SCNB model, it was necessary to create an accurate model of SENB test as well. The purpose of this model was the same as for the SCNB, to compare DEM results with lab tests and FEA results. Also, if similar tensile strength values were obtained from both SCNB and SENB DEM models this would further verify that either test can accurately produce the correct material properties.

Since SENB test is very similar to SCNB test, the development of this model was much easier. The only significant change between this model and the previous one was the arrangement of the elements in the model. For this test, a rectangular cross-section is used as opposed to the circular cross-section of SCNB test. This model incorporated a similar staggered stacking method as the one used for SCNB model for the purpose of decreasing the void space between elements and making the model resemble an actual HMA cross-section more accurately.

The micro properties used for this model were almost identical to those from SCNB model. The only difference was that the bond strength values were modified slightly. The left side of Figure 5 shows the completed SENB model and the propagation of the crack through the model. As with SCNB test simulation, the tensile stress at the notch tip was plotted and can be seen on the right side of Figure 5.

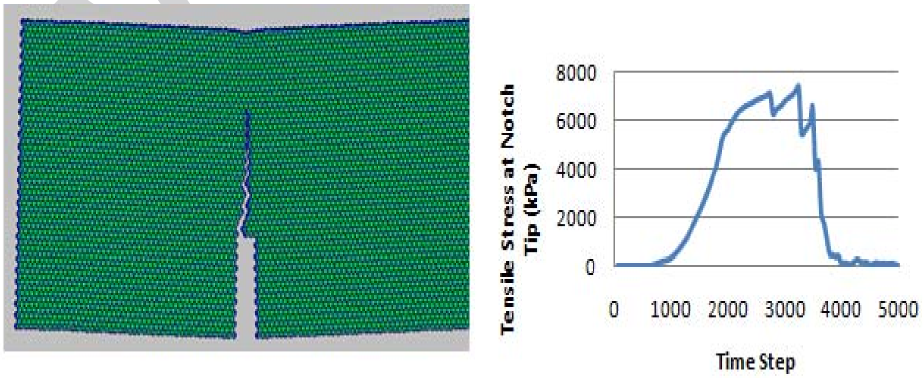

Figure 5. SENB model with crack and plot of tensile stress at notch tip

The earlier study by the authors [1] illustrated that both FEA and DEM models showed a good correlation between the SCNB and SENB models and demonstrated that either test will produce valid results. Also, the values calculated from the DEM analysis closely match those from the FEA analysis which along with the lab tests confirms the accuracy of the numerical analyses (as shown in Table 1).

Table 1: Numerical Analysis Results and Comparison for SCNB and SENB Tests [1]

Type of Analysis	**Tensile Stress at Crack Tip**		**% Difference**	K_{IC}		**% Difference**
	SCNB Test	**SENB Test**		**SCNB Test**	**SENB Test**	
FEA	8.07MPa	7.53MPa	7%	$9.1\text{MPa}\cdot\text{m}^{0.5}$	$8.7\text{MPa}\cdot\text{m}^{0.5}$	4.4%
DEM	7.69MPa	7.42MPa	4%	$8.7\text{MPa}\cdot\text{m}^{0.5}$	$8.6\text{MPa}\cdot\text{m}^{0.5}$	1.3%

3.3 Brittle Rock Model

The third model that was constructed for this study dealt with a completely separate area than the previous two HMA models. The purpose of this part of the study was to develop a DEM model to accurately reproduce the results of the shear failure testing on brittle rocks, specifically sandstone or granite. The goal of creating this model was to help civil engineers, miners, and geologists to better understand the mechanisms that cause shear failures in rock.

Understanding and preventing shear failures is important because they typically result in sudden, catastrophic collapses. The laboratory set up for this test is shown below in Figure 6. The test is performed on a 10 x 10 x 10 cm cube of rock and the contact points for applying the load are steel plates measuring 0.6 x 0.25 x 10 cm. This plate size was chosen because it caused minimal interference with sample loading conditions and prevented crushing.

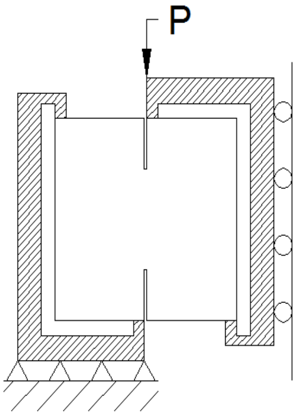

Figure 6. Brittle rock shear test configuration

For this model a similar approach was used as for the HMA models. The DEM model was constructed from rows and columns of small circular elements that were then bonded together, with contact bonds, to represent the rock specimen. As with the previous models the micro properties had to be estimated through trial and error. In the initial trials the lab dimensions were used for the steel loading plates, but even as the bond strength between elements was varied the results did not resemble those of the lab tests. Instead of observing a shear failure stretching from one notch tip to the other, the model tended to fail along a diagonal paths beginning at the outer edge of the steel plates and progress in towards the sides of the notches. A trial that resulted in this type of failure pattern is shown below in Figure 7.

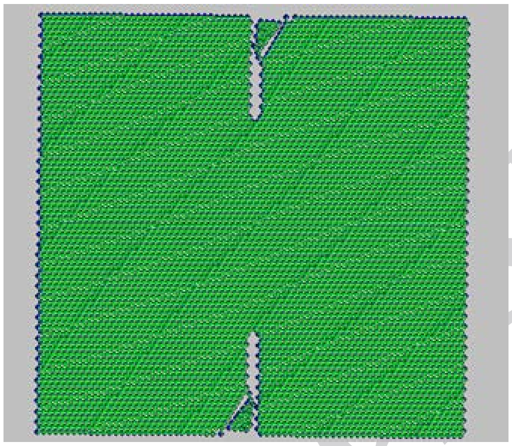

Figure 7. Inaccurate failure of shear model

In an attempt to avoid this erroneous solution, a model was constructed that used longer loading plates. Again multiple trials were conducted to find the best estimate of the micro properties for the model. The diagonal shear failures from the initial setup were not seen with this loading arrangement. However, after several iterations an accurate solution was not achieved. With this load configuration the model did not behave rigidly enough and the sample tended to buckle in towards the notches. An example of a model which failed in this manner is shown in Figure 8.

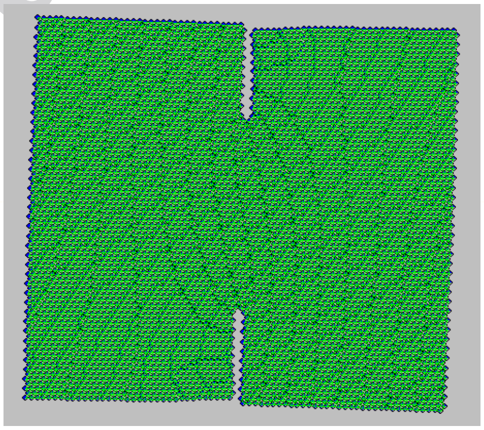

Figure 8. Alternate inaccurate failure of shear model

The previous result indicated that the use of contact bonds was allowing the elements within the model to rotate, which would not happen with a brittle rock specimen. To correct this error a new model was created that used parallel bonds instead of contact bonds. Unlike contact bonds, parallel bonds have an actual thickness, which prevents rotation between bonded elements. The trade off for creating a more rigid model is that there are more micro property values which must be correctly approximated to obtain useful results. In addition to bond strengths, bond stiffness must also be specified for parallel bonds. Various different combinations of values for the bond strength and stiffness (both shear and normal) were evaluated without reaching an acceptable solution. The results ranged between models that were very stiff and did not flex at all under relatively large loads and models that were so brittle that all of the bonds broke when the slightest load was applied. Due to these results it seems that a further investigation into the correct micro properties for brittle rock is necessary to create a functioning model. The capabilities of PFC2d software are more than sufficient to model this test setup but without a better understanding of the material properties, accurate results will not be obtained.

4. DEM VS. FEA

One of the reasons for conducting this analysis was to compare the effectiveness of DEM models for different scenarios versus existing FEA models. As discussed previously, for the HMA tests, the results from DEM models showed good correlation with the results from FEA models. One of the major advantages of DEM models for SCNB and SENB tests was that models particles were able to move. This allowed the nucleation and propagation of cracks to be observed. Another benefit of using a DEM model for HMA tests was the option to create particles of various sizes and place them in an arrangement that closely models actual HMA cross-sections. This can be achieved by clumping multiple small particles together as mentioned above. The main disadvantage of using DEM models that was observed during this study was the difficulty of determining the correct micro properties for materials that were modeled. If the necessary macro properties are known prior to the development of a model then this disadvantage can be mitigated by using equations (such as those provided by Yu et al. [23] for HMA) to convert the macro properties to micro properties that can be used in the model.

5. DISSCUSION AND CONCLUSIONS

The models created for this study demonstrated that the PFC2D software is a powerful analysis tool that can be adapted to a variety of scientific and engineering applications. The first two models created were used to verify the results of lab testing conducted on HMA specimens. Once correctly calibrated these models helped to prove that SCNB test was capable of producing results that matched those of SENB test. Also, DEM allows researchers to observe the processes that occur during crack propagation. The third model was developed for investigating shear failures of brittle rock and demonstrated one of the major disadvantages of PFC2D analysis. If the necessary properties of the material being evaluated are not well known it can make the development of an accurate model difficult and time consuming. Although, this model did not function properly with the correct material properties it would be possible to develop a working model for this test as well.

The two HMA models that already produced useful results can still be improved in several ways. By utilizing image processing and segmentation software, it would be possible to more accurately model existing HMA specimens used in lab testing. The improvement would also likely be coupled with the clump command in PFC2D software to create larger more angular elements to represent aggregates in the model. A second improvement would be to simplify the user interface through the development of an easy to understand simpler graphic user interface (GUI), thus, increasing the adoption of this software by a wider range of users.

Overall the PFC2D software has demonstrated to be a very useful tool for modeling several HMA laboratory tests and with proper modification it can also be adapted to modeling many other materials. One of the major advantages of using a DEM is that particles are free to move as opposed to a FEA model where everything is fixed in place and no separation of elements are allowed. For the applications of this study it meant that it was possible to observe the growth of cracks through the model. As software such as PFC2D become more accessible and understandable to a wider range of people, they have the potential to become a standard analysis tool in many science and engineering industries.

Although this paper represents the conclusion of this specific investigation into this study, it would be possible to further this research in several areas. The clearest way that the models could be enhanced would be to perform the necessary analysis to estimate the correct micro properties for each model. The equations for this process already exist so the only values that are needed are the required material properties from lab testing.

The second way in which the HMA models could be modified is to use the clumping process in the PFC2D software to create large angular elements that would more accurately approximate aggregates. The most useful way to employ this improvement would be to couple it with image processing and segmentation software. The purpose of using image processing and segmentation would be to generate model cross-sections that very closely resemble actual lab specimens. This can be achieved by importing a digital image of the actual sample into segmentation software, which would differentiate between mastic regions and aggregates. Once the segmentation software had separated out the different materials it would be possible to import the shapes into the PFC model. Then the clump command could be used to permanently bond adjacent particles together in the shape of the aggregates and mastic. Finally, different micro properties could be assigned to the areas of distinct materials.

A third addition that could improve the usefulness of the PFC models would be the development of a simpler graphic user interface (GUI) for variable input and results synthesis. In general the software is set up so that it can be adapted to most types of problems. Since the models discussed in the paper are for specific applications much of the code does not need to be visible for a casual user to benefit from the model. The simplified GUI would allow the user to input values for either the macro or micro properties of the model and if desired select the digital image to be modeled. Then the analysis could be run and the results presented in easy to access graphs and figures. The main advantage of software such as this would be that it makes the powerful analysis of DEM available to more users without the lengthy learning process.

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