Advances in micromechanical constitutive theories and modeling in asphalt mixture: A review

Jiantong Zhang\textsuperscript{a}, Jun Yang\textsuperscript{a}\textsuperscript{*}

\textsuperscript{a}School of Transportation, Southeast University, Nanjing, 210096, P.R. China

Abstract

An overview of the micromechanical constitutive theories of asphalt mixture is presented in this paper. Studies about constitutive theories and modeling methods are grouped into different categories: models with non-interacting particles (with and without geometry specified), models with particle interaction, finite element network models (FENM), micromechanical finite element models (FEM), clustered discrete element models (DEM), disturbed state concept (DSC), numerical manifold methods (NMM), and meshfree manifold methods (MMM) used in micromechanical modeling of asphalt mixture. Advantages, limitations and perspectives of different micromechanical approaches for the simulation of asphalt mixture are also analyzed. It is concluded that DEM and FEM are effective methods for particle scale research of asphalt mixture. The needs for future research are discussed as well.

Keywords: Asphalt mixture; Micromechanical modelling; Micromechanics; Microstructure; Finite elements; Discrete elements

1. Introduction

The size effect is a problem of scaling, which is central to every physical theory (Bazant, 1999). Scaling problems are even greater in road and railway. Asphalt mixture is a complex composite material made of aggregates, asphalt binder, and air voids. The performance of asphalt mixture is governed by properties of aggregate (shape, size distribution, modules, etc.), properties of asphalt binder (grading, complex modules, steady-state viscosity, asphalt modifiers, etc.), and asphalt-aggregate interactions (adhesion and absorption, etc.). With the goal to understand principal pavement distresses such as rutting, fracture, distortion, and disintegration, many models have been represented, such as viscoelastic, viscoplastic, and viscodamage constitutive model. Those models that considered the geometry of particles, the complex mixture microstructure and aggregate-aggregate interaction have been developed in recent years (You, 2007). Because of the limitation of traditional methods, combining with digital image processing and numerical simulation technology, X-ray

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Computerized Tomography (XCT) was used to study the microstructure of asphalt mixture for analyzing internal structure of asphalt mixture.

Within the last two decades, the stress–strain behavior of the asphalt mixture has been studied using two main approaches, one is macromechanical and the other is micromechanical (Abbas, 2007). In the macromechanical approach, a constitutive model is used to represent the composite behavior, whereas the model’s parameters are obtained through experimental measurements on representative samples of the composite. A wide range of constitutive relationships have been utilized for this purpose ranging from the simple elastic to the more elaborate elasto-visco-plastic material models (Sousa et al. 1993; Masad et al. 2005). The micromechanical approach, on the other hand, is based on discretizing the asphalt mixture microstructure and modeling the material properties of its constituents. The advantage of this approach is that it accounts for the material anisotropy and heterogeneity resulting from the aggregate shape and distribution within the asphalt mixture. Therefore, the discrete element method (DEM) is used to model the complicated viscoelastic behavior of asphalt mixture, which shows discrete behavior as relative positions of aggregate particles are changed during deformation.

The microscopic model considers the changes in the internal structures, properties of components, and interactions between aggregates and asphalt binder. Therefore, microscopic models of asphalt mixture include most of the important factors that govern the performance of asphalt mixture. Microscopic models based on DEM (Cundall and Hart 1990) can be adopted to study the behavior of asphalt mixture. Models based on DEM include fundamental theories such as linear or nonlinear contact laws at the microscopic level.

Micro-mechanics is one such area, in which mechanical behavior is described starting from the grain scale level, which relates microscopic parameters to macroscopic behavior. Modern research in this field resumed in the mid-1950s, using physical model experiments (Schneebeli, 1956; Dantu, 1957). More recently, works using numerical simulation with discrete element models (DEM) (Cundall and Strack, 1979) offers a unique opportunity to obtain complete qualitative information on all microscopic features of assemblies of particles.

2. Micro-macro Transition Approaches

Classical theories of plasticity failed to predict deformation in the post-critical regime because an internal length scale was not built into these constitutive relations. To capture post-critical behavior, microstructure is built into the constitutive relations. Figure 1 shows the process of micro-macro transition for prediction of asphalt mixture. During the integration process, a relationship is required to link the macro and micro-variables. Microstructure can be built into a deformation theory description by accounting for intergranular. The micromechanical parameters of asphalt concrete matrix include: (1) particle shape; (2) size and size distribution of particles; (3) concentration and concentration distribution of particles; (4) orientation of particles; (5) spatial distribution of particles; (6) composition of disperse phase; (7) composition of continuous phase, and; (8) bond between the continuous and disperse phases.

Microstructural models for more complex elasto-plastic behavior of granular material can be generally classified into two categories (An et al. 1994). The first category is plasticity models with fabric tensor, in which the material parameters of plasticity are defined at the macro (particle assembly) level. The second category is microstructural plasticity model, in which the material parameter is defined at the micro (inter-particle) level.
3. Numerical Techniques for Asphalt Mixture Micromechanics

Micromechanical models were recently developed to study the properties of heterogeneous asphalt mixtures (Papagiannakis et al., 2002; Li et al., 2005; Dai et al., 2006; You et al., 2007; Liao and Chang, 1992). Micromechanical models can predict fundamental material properties based upon the properties of the individual constituents such as the asphalt matrix and aggregate. The microstructure-based finite element and discrete element models were generally used to simulate the material constitutive behavior (Sepehr et al., 1994; Abbas et al., 2005; Sadd et al., 2005; Dai et al., 2007; Buttlar et al., 2001). The 2D and 3D micromechanical modeling of asphalt mixture were accomplished by incorporating viscoelastic elements for matrix and elastic body for each aggregate within a microstructure setting. Digital samples generated from X-ray CT images were used to predict the viscoelastic behavior of asphalt mixture. The material parameters of aggregates and matrix were measured and inputted to the models.

3.1. Digital technology application

The most recently research about microstructure of asphalt mixture focused on following two aspects: (1) quantitatively or qualitatively analyzing the internal structure of asphalt mixture; (2) based on one or several two-dimensional numerical models were established for mechanics simulation. It is obvious that the research is limited. X-ray CT imaging is an advanced technique for acquiring a stack of sectional images within heterogeneous materials. Compared to optical imaging approaches, X-ray CT has the advantage of acquiring accurate digital information of the internal microstructure and 3D geometry of solid objects in a non-destructive manner. Digital specimen and test techniques permit investigation of strength and deformation mechanisms of asphalt concrete in a microscopic way that integrates mechanism identification, numerical simulation, and experimental observations. It represents the trend for the future mix design (Robert, 2002).

For microstructure acquisitions, planar X-rays were projected directly along the circular cross-section of material specimens. As the specimen rotates 3600 under the planar X-ray projection, the CT numbers were obtained at all directions. With these collected CT numbers, the surface slice image was captured. To obtain 3D internal microstructure, the specimen was shifted vertically with an interval distance. Thus the surface images at
different heights with the equal interval were captured, and these images were stacked to reconstruct the 3D microstructure of the specimen. Masad (2005) developed a new method AIMS (Aggregate Imaging System) that is capable of directly measuring the characteristics of coarse and fine aggregates.

3.2. The two-dimensional and three-dimensional digital reconstruction of asphalt mixture

The challenges in the modeling of asphalt mixture contain the highly heterogeneous nature including aggregate internal structure and air void distribution, the time, temperature and rate-dependent behavior of the matrix and the limited computation capacity for very precise prediction. Many researchers presented the two-dimensional and three-dimensional (2D and 3D) micromechanical FE models for predicting the viscoelastic properties of heterogeneous asphalt mixture. To reconstruct the asphalt mixture, its microstructure and material parameters should be known. The microstructure of material specimens is captured with the non-destructive X-ray CT imaging techniques. Then, the material parameters of elastic aggregates and viscoelastic matrix are determined from the lab test data. Dai (2011) reconstructed 2D and 3D structure of asphalt mixture using micromechanical finite element (FE) models to predict the viscoelastic properties. The micromechanical FE model was accomplished by incorporating the captured microstructure with X-ray computed tomography imaging techniques and ingredient properties (viscoelastic asphalt matrix and elastic aggregates). You (2012) presented a 3D microstructure-based computational model to predict the thermo-mechanical response of the asphalt concrete using a coupled thermo-viscoelastic, thermo-viscoplastic, and thermo-viscodamage constitutive model. The 3D microstructure of the asphalt concrete was reconstructed from slices of two-dimensional X-ray computed tomography images that consist of the matrix and the aggregate phases and ignoring voids.

Chang and Meegoda (1997) described different types of aggregate-aggregate and asphalt-aggregate contacts. The viscoelastic behavior of the asphalt binder was described using the Burger model (see Table 1.). In this model the asphalt mixture specimen was reconstructed with a given number of aggregates coated with asphalt cement. The asphalt cement is microscopically represented by two sets of viscoelastic elements in normal and tangential directions at each contact. The number of viscoelastic elements for a given specimen depended on the number of asphalt-coated aggregate contacts. The aggregates in contact were represented by a mass with a moment of inertia connected by viscoelastic elements in the normal and tangential directions at each contact. Each contact is either an aggregate-asphalt-aggregate contact or an aggregate-aggregate contact.

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<thead>
<tr>
<th>Contact types</th>
<th>Contact model</th>
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</thead>
<tbody>
<tr>
<td>Interactions within aggregates</td>
<td>Contact-stiffness model</td>
</tr>
<tr>
<td>Interactions within sand mastic</td>
<td>Contact-bond model + Burger’s model</td>
</tr>
<tr>
<td>Interactions between aggregate and sand mastic</td>
<td>Contact-bond model + Burger’s model</td>
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3.3. Discrete element methods of asphalt mixture

Discrete element models can be used to model dynamic or quasi-static systems. Generally speaking, the modeling progress is showed as Fig. 2. Modeling of asphalt concrete can be considered as quasi-static problems. The equation of motion for each particle is expressed as

\[ M\ddot{x} + D\dot{x} + R(x) = F \]

Where \( \ddot{x}, \dot{x}, x \) = linear acceleration, velocity, and displacement vector, respectively; M=mass; D=damping; R=internal restoring force; and F= external force.
In DEM modeling, 2D and 3D virtual structure of asphalt mixture can be reconstructed using the software of PFC2D or PFC3D. Rotherburg et al. (1992) studied the interaction between idealized representations of elastic aggregates using a viscoelastic contact model. It was concluded that the complex behavior of the granular matrix is the main reason for nonlinear trends in the mechanical response of asphalt mixtures and, to a larger degree, its susceptibility to rutting. An increase in the mix strength was reported due to the increase in aggregate angularity.

The DEM can be utilized to study the effect of repeated loading on permanent deformation and fatigue failure of asphalt mixture (Ullidtz, 2001). Aggregate angularity and particle size distribution were controlled in the analysis through the use of multisided polygons of different sizes. DEM was used to simulate the indirect tension test (Buttlar and You, 2001). Particle interaction was described using a linear elastic contact model. The geometry was defined using a more realistic procedure based on two-dimensional images of the asphalt mixture microstructure. It was concluded that the 2D DEM models over predicted the specimen deflection as a result of not taking into account the actual interlocking among aggregates, which is present in the three-dimensional physical specimen. The same approach was used to simulate the hollow cylinder tensile test with the objective of studying the effect of the wall thickness and the size of the surface voids on the measured asphalt mixture complex modulus (Buttlar et al. 2004).

In summary, DEM was found to be an excellent tool to investigate the influence of aggregate characteristics on the performance of asphalt mixtures because it can simulate the micro-mechanical behavior of granular materials. In particular, aggregate shape and angularity were found to be amongst the most important parameters that affect asphalt performance as they have a strong influence on the way which grains make contact and interlock. It should be noted that in the DEM simulation it is almost impossible to take the fine particles fully into consideration because not only this significantly increases computational time and cost, but it also affects the system’s capability to reach equilibrium.

3.4. Micromechanical finite element modeling approach

The FE modeling of asphalt concrete allows accurate prediction of mixture properties by incorporating aggregate and matrix constitutive behaviors and microstructure geometries. The digital sample contains the real microstructure obtained from X-ray CT images including irregular aggregates, asphalt matrix and air voids. The
FE meshes of these samples were generated from the image pixels. The micromechanical modeling scheme combines the matrix elements with specially-defined viscoelastic behavior and elastic aggregate bodies. The material parameters of asphalt matrix and aggregates were determined from the lab test data.

In finite element modeling, photographic and X-ray computed tomography images were used to describe the internal structure of asphalt mixtures (Kose et al., 2000). Masad et al. (2002) utilized image analysis techniques and FEM simulations of the microstructure to study the stiffness anisotropy of asphalt mixtures. Masad et al. (2002) and Papagiannakis et al. (2002) presented a procedure to process an asphalt mixture image for modeling purposes. Due to resolution limitations in capturing and processing asphalt mixture images, it was found that the image binder thickness was larger than the actual film thickness. Further, the smallest microstructure element (image pixel) did not represent binder only but also the fine particles embedded in the binder (i.e., this agglomerate being referred to as mastic). To account for these two factors, it was necessary to multiply the measured binder stiffness by a factor to obtain the stiffness of the mastic. Nonlinear viscoelastic material model incorporated in the FEM to analyze the asphalt mixture microstructure (Abbas et al., 2004). The model geometry was described using the same procedure presented by Papagiannakis et al. (2002). The viscoelastic behavior of the asphalt mastic was defined using a nonlinear viscoelastic material model, which was numerically solved using a convolution integral approach. To account for the asphalt binder nonlinearity, the mechanical parameters were updated during the analysis according to the strain level within each element. Computational micromechanics modeling approach was used to predict damage-induced mechanical response of asphalt mixtures (Kim et al., 2005). Heterogeneous geometric characteristics and inelastic mechanical behavior were taken into account by introducing finite element modeling techniques and a viscoelastic material model. The modeling also included interface fracture to represent crack growth and damage evolution. The interface fracture was modeled using a micromechanical nonlinear viscoelastic cohesive-zone constitutive relation.

3.5. Modeling microstructure of asphalt mixture

The microstructural features of aggregate include: mineralogy, elastic modulus, size, shape, texture and packing geometry. The full description of micromechanical behavior may be divided into three points: (1) structure (position of grains and contacts between them); (2) the kinematics evolution (displacements, rotations, evolution of contacts); (3) intergranular forces.

A relationship should exist among these micromechanical features which dictate the macroscopic behavior. Micro-mechanics is the science in which these micro-macro relationships are developed by averaging techniques over a group of particles based on statistical mechanics principles. Micromechanics deals with the relationship between external stresses and strains, and average internal forces and displacements. In a continuum, the stress is defined as the force per unit area. In a two-dimensional case, this reduces to the force acting on a unit line. In the case of a particulate system, the above definition needs a suitable averaging technique. The search for explicit relationships between stress tensor and parameters that describe interparticle forces and fabric has been the subject of number of researchers beginning with the work of Dantu (1957) and Sitharam (2000).

To relate micromechanical characteristics to macroscopic behavior, fabric description is an essential element. Fabric is a quantity whose importance is well known. However, methods to quantify it are not very well established. The presence or a fabric term in the relationships between force and stress, and similarly between displacements and strain in particulate medium can be easily visualised. Quantification of fabric requires knowledge of the number of contacts in a representative volume and also the distribution of contact orientations for the purpose of relating average forces to stress, and displacements to strains. In this direction, experimental work with assemblies of discs made of optically sensitive materials has provided a better understanding of micro-macro relationships and the fabric (Richard et al., 2004; Oda et al., 1989; Buttlar and You, 2001).

Detailed microscopic information on a numerically simulated assembly of discs can be used to trace the evolution of microstructure and contact forces during shear deformations. Rothenburg and Bathurst (1989) shown that the macroscopic stress can be related to microscopic force and fabric parameters by following expression.
Where $\sigma_{ij}$, $m$, $E$ are the macroscopic stress, contact density, assembly average contact vector length, distribution of average normal contact force, distribution of average shear contact force, contact normal vector, contact shear vector, and contact normal distribution function, respectively.

Heterogeneity can be included in lattice models through two approaches, microstructure-based and statistics-based. In the first approach, a (regular) lattice mesh is projected onto the actual material structure and the properties of each lattice link are assigned according to the material that the link lies over. The second approach is to translate the microstructural information into a statistical distribution that is subsequently used to assign strength and stiffness properties to different lattice links. In the second approach, the lattice system is less refined than the first approach, but more phenomenological and the reported 2D analyses show large deviation from reality. Feng (2003) developed a new microstructure-based approach that the lattice mesh was directly transformed from the configuration of aggregate particles, instead of projecting the mesh onto the microstructure.

It should be noted that most models have been developed based on macrostructure measurements, assuming asphalt mixture to be isotropic, and ignoring the mechanisms that are in playing at the microstructure level. Tashman et al. (2005) presented a microstructure-based viscoplastic continuum model which was developed for the permanent deformation of asphalt concrete. Based on the continuum damage mechanics, a general and comprehensive thermodynamic-based framework for coupling the temperature dependent viscoelastic, viscoplastic, and viscodamage behaviors of bituminous materials was presented by Darabi (2011). This general framework derived systematically Schapery-type nonlinear viscoelasticity, Perzyna-type viscoplasticity, and a viscodamage model analogous to the Perzyna-type viscoplasticity.

To develop a microstructure-based continuum model for AC permanent deformation is a pressing need. The model can account for the phenomena influencing permanent deformation including the effect of the microstructure in terms of the anisotropy of aggregate distribution and damage in terms of crack and air void growth. Anisotropy is caused by the non-uniform directional distribution of microstructure quantities such as contact normals, particles orientation, void orientation, or branch vectors. An anisotropic viscoplastic continuum damage model was developed by Tashman et al. (2005) to describe the permanent deformation of asphalt pavements. The model was based on Perzyna’s theory of viscoplasticity with Drucker-Prager yield function modified to account for the microstructure anisotropy and damage. X-Ray computed tomography and image analysis techniques were used to capture and characterize the evolution of cracks and air voids in the deformed specimens. Masad (2007) developed an elastoviscoplastic model that accounted for the influence of important microstructure properties such as anisotropy based on particle orientation distribution and damage on permanent deformation.

The contact normal is defined as the vector normal to the tangent plane at the point of contact between particles. A particle orientation is defined by the direction of the longest axis of a non-spherical particle. A branch vector is represented by a line joining the centers of mass of the contacting particles. The directional distribution of voids is described by dividing the void space to a number of “unit voids”, and assigning a vector to describe the orientation of each unit void. The orientation tensor on the other hand, remains almost unchanged even at later stages of deformation (Oda et al., 1985; Oda and Nakayama, 1989).

Masad et al. (1998, 1999) and Tashman et al. (2001) developed image analysis techniques (IAT) to quantify the microstructure of AC in terms of aggregate orientation, aggregate gradation, aggregate contacts, aggregate segregation, and air void distribution. These techniques can be easily implemented to quantify the anisotropy of the aggregate orientation in two-dimensional cut sections of AC. Oda and Nakayama (1989) expressed the microstructure tensor as a function of an anisotropy parameter, known as the vector magnitude $\Delta$ as follows:

$$F_\theta = \begin{pmatrix}
\frac{(1 - \Delta)/(3 + \Delta)}{0} & 0 & 0 \\
0 & \frac{(1 + \Delta)/(3 + \Delta)}{0} & 0 \\
0 & 0 & \frac{(1 + \Delta)/(3 + \Delta)}
\end{pmatrix}$$
Where $\Delta$ is a microstructure parameter that quantifies the average anisotropy of the aggregate orientation distribution measured on two-dimensional axial cut sections of the material as follows:

$$\Delta = \frac{1}{M} \left[ \left( \sum_{k=1}^{M} \cos 2\theta^k \right)^2 + \left( \sum_{k=1}^{M} \sin 2\theta^k \right)^2 \right]^{\frac{1}{2}} \quad (4)$$

Where $\theta^k$ is the orientation of an individual aggregate on a two-dimensional image of a cut section ranging from -90° to +90°, and M is the total number of aggregates analyzed in an image.

Oda and Nakayama (1989) incorporated the microstructure tensor $F_{ij}$ in the Drucker-Prager yield function. Based on Perzyna’s theory of viscoplasticity with the Drucker-Prager yield function modified to account for the microstructure anisotropy and damage, micromechanical constitutive of asphalt mixture can be built. X-Ray computed tomography and image analysis techniques were used to capture and characterize the evolution of cracks and air voids in the deformed specimens (Tashman et al., 2005). Digital specimen and test techniques permit investigation in strength and deformation mechanisms of asphalt concrete in a microscopic way that integrates mechanism identification, numerical simulation, and experimental observations. It represents the trend for the future mix design (Robert, 2002).

### 3.6. Numerical methods for modeling discontinuous

The commonly used methods to numerate discontinuous mechanics mainly include DEM (Discrete Element Method), DDA (Discontinuous Displacement Analysis), and NMM (Numerical Manifold Method). Among these methods, DEM is the most successful to be applied for asphalt mixture, it is a mature method in solving the discontinuous problems and large deformation cases. However, because DEM tightly depends on combination of elastic or viscous components to reflect the contact state between particles, it hardly achieves stress distribution of asphalt mastic(Zhou, 2009).

NMM was established by Shi Genhua (1991 and 1997) by using finite covering system in modern manifold, it takes advantage of finite element method and continuum kinematics, combines discontinuous and continuous deformation into a uniform mathematical expression. In theory, Meshfree Manifold Method (MMM) is good at dealing with discontinuous problems of asphalt mixture, especially for large deformation, cracks, and material coupling calculation.

The disturbed state concept (DSC) provides a modeling approach that includes various responses such as elastic, plastic, creep, microcracking and fracture, softening and healing under mechanical and environmental (thermal, moisture, etc), within a single unified and coupled framework (Desai, 2007). Although the DSC can provide a unified model for pavement materials, its limitation may arise due to the lack of appropriate and (laboratory) test data for its calibration, and due to the lack of comprehensive field measurements for its validation.

### 4. Conclusions

When analyzing the microstructure and micromechanics of asphalt mixture, a number of challenges have to be overcome, need to expand our understanding of micromechanical models. This paper presents an overview of the work done by many researchers on the micromechanical constitutive theories and modeling of asphalt mixture. The recently developed methods used in micromechanical modeling of asphalt mixture, such as finite element network model (FENM), micromechanical finite element model (FEM), clustered discrete element model (DEM), disturbed state concept (DSC), numerical manifold method (NMM), meshfree manifold method (MMM) are also described. More and more researchers have studied the microstructure of asphalt mixture using XCT. It is believed that a number of research works of micromechanical modeling technique will be presented for designing asphalt mixture in the future.
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