

MODELING OF ASPHALT DURABILITY AND SELF-HEALING WITH DISCRETE PARTICLES METHOD

V. Magnanimo, H. L. ter Huerne and S. Luding

Tire-Road Consortium, CTW, University of Twente, Netherlands – corresponding author: v.magnanimo@utwente.nl

ABSTRACT

Asphalt is an important road paving material. Besides an acceptable price, durability, surface conditions (like roughening and evenness), age-, weather- and traffic-induced failures and degradation are relevant aspects. In the professional road-engineering branch empirical models are used to describe the mechanical behaviour of the material and to address large-scale problems for road distress phenomena like rutting, ravelling, cracking and roughness. The mesoscopic granular nature of asphalt and the mechanics of the bitumen layer between the particles are only partly involved in this kind of approach. The discrete particle method is a modern tool that allows for arbitrary (self-)organization of the asphalt meso-structure and for rearrangements due to compaction and cyclic loading. This is of utmost importance for asphalt during the construction phase and the usage period, in forecasting the relevant distress phenomena and understand their origin on the grain-, contact-, or molecular scales. Contact models that involve visco-elasticity, plasticity, friction and roughness are state-of-the art in fields like particle technology and can now be modified for asphalt and validated experimentally on small samples. The ultimate goal is then to derive micro- and meso-based constitutive models that can be applied to model behaviour of asphalt pavements on the larger macro-scale. Using the new contact models, damage and crack formation in asphalt and their propagation can be modelled, as well as compaction. Furthermore, the possibility to trigger self-healing in the material can be investigated from a micro-mechanical point of view.

Keywords : discrete element modeling, mastic asphalt, material behavior, continuum methods

1. INTRODUCTION

Asphalt mixtures are composite materials that consist of solid particles, viscous binder/fluid (bitumen) and pores filled with air. When considering asphalt we should distinguish different states the mixture can be in: a) hot and non-compacted (construction phase, relatively loose particle matrix) and b) compacted at ambient temperature. During compaction of the mixture the relative contents of the different phases changes: starting from the initially loose material, the particles in the skeleton move close to each other and air in the voids is squeezed out. The fluid in the mixture (that can be hot or cold, i.e. less or more viscous) lubricates the contact surfaces between the particles and can make movement of the particles easier [1]. The multiphase material has properties that depend on those of the original components, i.e. aggregate and binder. The physical properties of the skeleton (e.g. shape, surface texture, size distribution, moduli), but also the properties of the binder (e.g. grade, relaxation characteristics, cohesion) and binder–aggregate interactions (e.g. adhesion, absorption, physiochemical interactions) characterize the material behavior of the asphalt mixture. In addition, aggregate particles in the mixture have different shapes, surface texture and orientations, which make the description of the contacts between particles a challenge [2].

When looking at asphalt, it makes sense to distinguish between three different length scales, i.e. micro-, meso- and macro-scale. The interaction between the mortar (composition of bitumen and the smallest particles) and a single large stone is defined as the micro-scale. The interaction of multiple stones of various sizes and the mortar is defined as the meso-scale. On the macro-scale, the behavior of the whole road is accounted for. Kinematics at different scales apparently governs the behavior of the material: to gain thorough knowledge of asphalt pavement behavior, one has to focus on all three length scales. As common practice in the professional asphalt branch, fundamental constitutive models able to describe the micro- and meso-mechanical behavior are hardly used. Large scale problems are addressed by using empirical models [1] for road distress phenomena like rutting, raveling, cracking and roughness. The mesoscopic granular nature of asphalt, the chemistry and the mechanics of the (modified) bitumen layer between the particles is, because of the limitations of those empirical models, just partly involved. Our ambitious goal is to bridge the gap between discrete and continuous concepts. The material behavior at the grain-scale can be combined with the granular structure in order to identify the contact law for the asphalt components and relate such kinematics with the macroscopic response at the larger scale of the road. Finding a micro-based model with predictive quality on the macro-level is the ultimate challenge.

On the particle-scale, the interaction of the mortar with the grains and between the grains can be efficiently investigated using a Discrete Element Method (DEM) [3]. Discrete element methods simulate particulate systems by modeling the translational and rotational degrees of freedom of each particle using Newton's laws, and the forces are calculated associating proper contact models with each particle contact.

In the last twenty years, attempts for a micro-mechanical modeling of asphalt have been done by other researchers: a contact law for the behavior of two particles connected by a binder and elastic to describe the behavior of an assembly of bonded particles was proposed in Ref. [4]; a micro-mechanical description of rutting with intergranular and aggregate-binder interactions was given in Ref. [5]; 2D modeling based on image processing are reported in [2]. DEM studies on cemented particulate materials include the work by Rothenburg et al. [5], Chang and Meegoda [6], Sadd and Dai [7], Buttlar and You [8] and Ullidtz [9].

Special attention deserves the Finite Element numerical approach LOT (Lifetime Optimization Tool) used in [10]. Here the authors define an adhesive zone, taking into account the boundary effect of the mortar. The stone chippings are modeled as pure rigid bodies, that can't deform. It is assumed that for modeling raveling, caused by repeated traffic loading, the effect of the bonding agent (mortar) is dominant. For this reason, they study cohesive failure (within the mortar) and adhesive failure (between mortar and stone chippings). Given the behavior of the mortar as input information from specific laboratory tests (Dynamic Shear Rheometer, Dynamic Material Analyser, Direct Tension Test), the adhesive zone can be reproduced. The mortar is modeled as a linear visco-elastic material. On the basis of the performed tests, a damage model for the adhesive zone is derived, and from here, input parameters for the LOT calculations are retrieved. Three types of FE model have been developed: i) 2D idealized, i.e. ideal 2D round particles; ii) 3D idealized, i.e. ideal 3D round particles, and iii) 2D photo/scan, based on pictures of real samples. FE simulations lead to the visualization of stress distributions in the sample. In Figure 1 the maximum principal stress within the mortar using the 2D photo/scan model is shown.

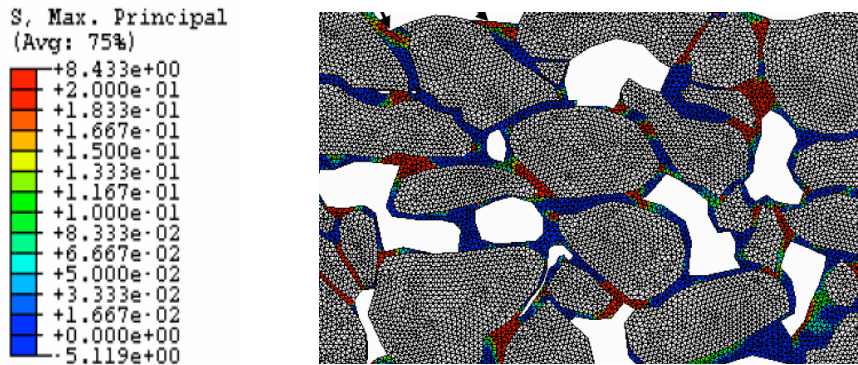


Fig. 1: Indication of the maximal principal stress (i.e. tensile stress) in the central area of the model (after [10] with thanks to the authors).

Nevertheless, a well-established multiscale description for the constitutive behavior of particle-bitumen systems is still missing. Particularly, very limited work has been done on 3D micro-mechanical modeling of the mixture, with proper visco-elasto-plastic, temperature-dependent contact/interaction models. Moreover, to our knowledge, no systematic numerical study on the microscopic processes that govern cracks (and eventually self-healing) in asphalt has been done. On the technological/methodological side, a general computational framework suitable for simulating the loading/cyclic and fracture/healing behavior of granular-bitumen composites is the need of the hour. The detection and analysis of damage as well as microscopic self-healing mechanisms have been achieved by particle based simulations already [11][12] so that these results now can be applied to asphalt and translated to a practicable continuum model with predictive quality, which will allow proposing and designing optimized materials with superior self-healing capabilities in the future [13].

In this preliminary study an approach to modeling of cohesive, sintering and self-healing particulate materials is described [14]. The mechanical evolution in time of all the particles in the material is simulated in DEM using a modern version of the sintering contact model [11]. This contact model mimics the physical behavior of the interaction of the particles accounting for dissipative, elasto-plastic, adhesive, and frictional effects and the pressure dependence. The model is by construction non-linear in its response to external load [11]. An additional temperature-dependence, as possibly resulting from diffusion of atoms and the resulting sintering effects, can be added on top of the elasto-plastic contact model [12].

Initially, some particle-samples are prepared by applying isotropic (hydrostatic) pressure. The spherical particles deform plastically at contact and stick to each other forming a solid sample with (after releasing pressure) zero confining stress – on which uni-axial tension or compression is further applied. The numerical results are compared (qualitatively) with laboratory uni-axial tests from [15] on samples of dense asphalt concrete. The comparison is encouraging as the model is able to reproduce the typical softening behavior of asphalt under compression.

Large deformations of sintered samples will then lead to damage. In the final part of the work, self-healing of sintered particulate materials is studied using the DEM simulations. Loose particles can sinter due to their time-, stress- or temperature-dependent contact properties and forces. Self-healing of damaged samples can be activated through re-sintering, a process that globally increases further the contact adhesion between particles. The simplest self-healing of particle contacts only involves the increase in contact strength due to re-sintering, without accounting in detail for all microscopic mechanisms. Experimental and numerical studies indicate that the net increase in strength depends on the sintering temperature and duration, see for example [12][16][17]. In the simulations, during the initial pressure sintering preparation, the optimal strength is not reached. Hence, the sample still has the potential to be strengthened further during a *second* sintering (healing). If the re-sintering is applied after the sample has already experienced some damage under mechanical loading (like uni-axial tension or compression), the question is to which extent the damage can be healed.

In Section 2 the technical details of the simulation method are summarized, and the pressure-sintering contact model is described. In the following section 3, numerical results of DEM simulations are reviewed for damage under unconfined uni-axial tensile and compressive loading. In Section 3.3 a qualitative comparison is made between the numerical data and results from laboratory uni-axial compression tests on unconfined asphalt samples [15]. In Section 3.4, DEM simulations are reported, where self-healing through re-sintering is applied to the previously used numerical samples. Finally in section 4, an example is reported describing how the parameters obtained from numerical element tests can be implemented in FE simulation to reproduce macro-scale asphalt processes.

2. SIMULATION METHOD

2.1 DEM modeling of particulate materials

The Discrete Element Method (DEM) [3] for particle systems can be used to illustrate how the macroscopic response of a solid-like, sintered sample, resembling an asphalt mixture, depends on various micro- and meso-scopic properties such as the particle-particle contact network, the particle size, and the contact adhesion between particles (simulating the interaction of the bitumen with the particles), their contact friction and stiffness. In the present work, after solving the equations of motion at the particle level, the coupling between micro- and macro scale properties is performed. The response of the particle system (expressed in terms of macroscopic stress and strain) is obtained by averaging [18] the local quantities at the particle contact level (interparticle contact forces and displacements) over the assembly. The effective response then depends directly on the chosen particle contact model [11][19][20]. Even though recent studies have demonstrated that the accurate simulation of systems composed of non-spherical particles is possible [21][22], for simplicity we restrict ourselves here to spherical particles.

2.2 Adhesive contact model

In the following, particulate material samples are (i) *prepared*, (ii) *deformed* and *damaged*, and then (iii) *self-healed* and (iv) *deformed* again. The non-linear model by Luding *et al.* [11][23][24] is used – see these references for more details, to describe the adhesive particle-particle interaction in the asphalt mixture. In Figure 2, the normal contact force f (that is directed parallel to the line connecting the centers of two contacting particles) is plotted against the contact overlap (resembling the deformation between particles at the contact), $\delta > 0$. If $\delta < 0$, there is no contact between particles, and thus $f = 0$. This sign convention relates positive (*negative*) values of the contact displacement δ to overlap/deformation (*separation*), while positive (*negative*) values of the contact force f relate to compression/repulsion (*tension/attraction*).

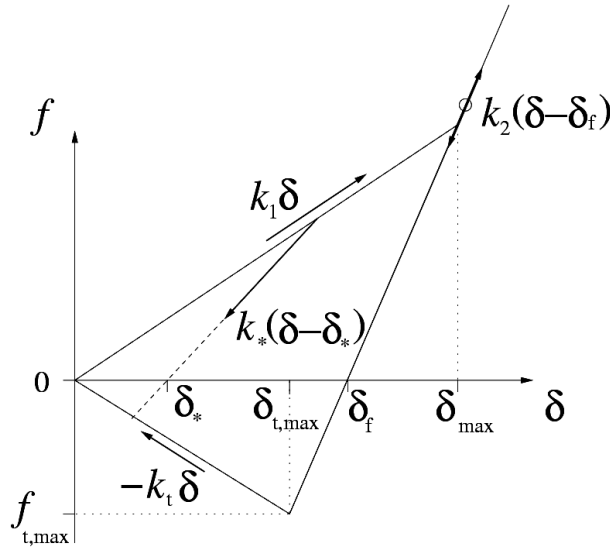


Fig. 2: Particle contact model plotted as force-displacement relation [11][23], with d for contact positive, and repulsion and attraction forces positive and negative, respectively.

A contact begins at $\delta = 0$ and, during initial compressive loading, the contact force increases with the overlap as $f = k_1 \delta$, with k_1 the elasto-plastic contact stiffness. When the external compressive forces are compensated by the contact repulsive force at the maximum contact overlap, δ_{\max} , for unloading, the contact stiffness increases to a value k_2 , so that the elastic unloading force is $f = k_2 (\delta - \delta_f)$. Elastic unloading to zero contact force leads to the (plastic) contact overlap $\delta_f = (k_2 - k_1) \delta_{\max} / k_2$. If the overlap is further decreased, the contact force gets tensile, with maximum tensile contact force $f_{t,\max} = -k_t \delta_{t,\max}$, realized at contact displacement $\delta_{t,\max}$.

For the sake of brevity, the tensile softening parameter k_t hereafter is referred to as the “contact adhesion”. Note that, mostly for practical reasons [11], for contact deformations above δ_{\max} , the force follows the limit branch $f = k_2 (\delta - \delta_f)$, since further loading is unrealistic anyway and would lead to much stiffer behavior if properly modeled. The extreme loading and unloading limit branches are reflected by the outer triangle in figure 1. Starting from the realized maximal overlap, $\delta_{\max}^* < \delta_{\max}$, unloading occurs within the outer triangle, as characterized by a branch with stiffness $k_* = k_1 + (k_2 - k_1) \delta_{\max} / \delta_{\max}$, and (elastic, reversible) force, $f = k_* (\delta - \delta)$. The intermediate stiffness k_* follows from a linear interpolation between k_1 and k_2 – which is our (arbitrary) choice due to the lack of experimental data on this (probably) non-linear behavior. In summary, the model has three (“stiffness”) k -parameters that describe the three relevant physical

effects at the contact: (1) elasticity, (2) plastic deformations, and (3) contact-adhesion. Furthermore, the model involves (4) a non-linear contact stiffness via the choice of k_* . This piece-wise linear model is a compromise between simplicity and the need to model physical effects. Except for some early theoretical studies, see [20] and the many works that are based on it, there is no experimental/numerical literature available to our knowledge that provides enough detailed information on the force-displacement relations, involving all four physical contact properties above and their nonlinear, history-dependent behavior. If this information becomes available, the present model can be extended and generalized.

The *tangential contact force* acts parallel to the particle contact plane and is related to the tangential contact displacement through a linear elastic contact law, with the tangential stiffness k_s . The tangential contact displacement depends on both the translations and rotations of the contacting particles. Coulomb friction determines the maximum value of the tangential contact force: During sliding the ratio between the tangential contact force and the normal contact force is assumed to be limited and equal to a (constant) dynamic friction coefficient μ_d ; during sticking, the tangential force is limited by the product of normal force and static coefficient of friction μ_s .

Tab. I: Microscopic material parameters based on Ref. [11], but rescaled as indicated in the right column.

| Property | Symbol | Values [14] | SI units |
|----------------------|------------------------|---------------------|-------------------------------------|
| Time Unit | t_u | 1 | 1 ms |
| Length Unit | x_u | 1 | 1 m |
| Mass Unit | m_u | 1 | 1 kg |
| Average radius | \bar{R} | $0.5 \cdot 10^{-3}$ | 0.5 mm |
| Material density | ρ | 2000 | 2000 kg/m ³ |
| Elastic stiffness | $k = k_2$ | $5 \cdot 10^4$ | $5 \cdot 10^{10}$ kg/s ² |
| Plastic stiffness | k_1 / k_2 | 0.5 | |
| Adhesion “stiffness” | k_i / k_2 | [0, ..., 20] | |
| Friction stiffness | k_s / k_2 | 0.2 | |
| Plasticity range | ϕ_f | 0.05 | |
| Coulomb friction | $\mu = \mu_d = \mu_s$ | 1 | |
| Normal viscosity | $\gamma = \gamma_n$ | $5 \cdot 10^3$ | $5 \cdot 10^6$ kg/s |
| Tangential viscosity | γ_f / γ | 0.2 | |
| Background viscosity | γ_b / γ | 4 | |
| Background torque | γ_{br} / γ | 1 | |

3. RESULTS: LOCAL BEHAVIOR

The simulations reported here consist of four subsequent stages, namely (i) a sample preparation stage (isotropic compression), (ii) an uni-axial (tensile or compressive) loading stage, (iii) a self-healing stage, and (iv) the continuation of the uni-axial loading.

Six plane, perpendicular outer walls form a cuboidal volume, with side lengths of $L = 11.5$ mm. The samples are composed of about 10^3 poly-disperse spherical particles (see Figure 3 as an example), with particle radii drawn from a Gaussian distribution around mean $\bar{R} = 0.5$ mm [11][25]. The particle density used in the simulations is $\rho = 2000$ kg/m³,

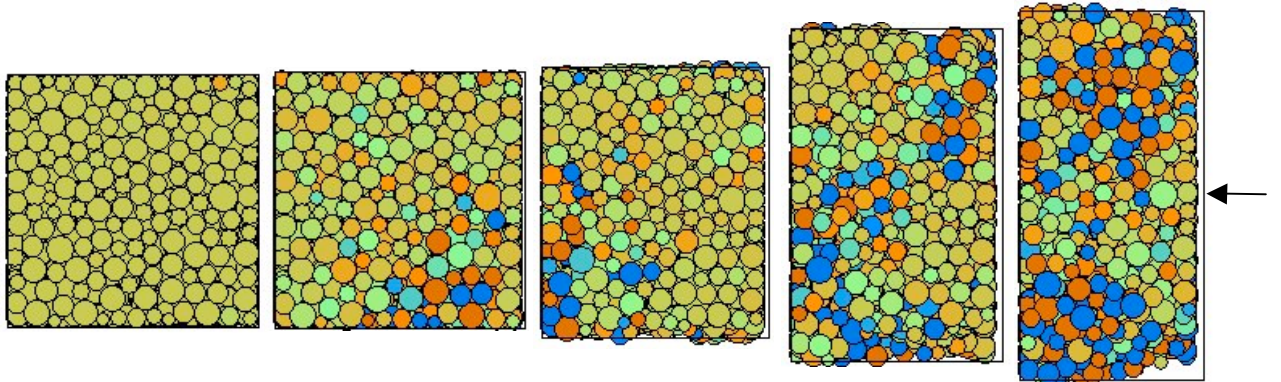


Fig. 3: Sequence of snapshots from a compression test with poly-disperse particles and rigid outer walls ($k_1/k_2=0.5$). The circles are the particles with the greyscale coding the average stress.

the maximum elastic contact stiffness is $k_2=5.10^{10}$ N/m. The initial elasto-plastic stiffness (normalized by k_2) is $k_1/k_2=1/2$, and the contact adhesion k_t/k_2 is varied. The other stiffness parameters, friction coefficients, and viscous damping parameters are summarized in Table I, most of them being dimensionless, like all quantities discussed in the rest of the paper. As final remark, we note that the choice of parameters is empirical – most of them kept fixed here, only adhesion is varied systematically.

3.1 Isotropic Loading

In this section the sample preparation by *pressure sintering* [23] is reported. During sintering, the particles deform plastically at contact and stick to each other due to strong, non-linearly increased van der Waals forces. At the same time, the sample shrinks, i.e. becomes denser. Such pressure-sintering results in a solid sample with bonded particles, similar to asphalt mixtures. Moreover, the sintering model can be temperature-dependent, resembling the effect of the temperature in the asphalt preparation with bitumen [12]. The process is characterized by two stages: the first stage reflects the application of a hydrostatic (or isotropic) pressure, $\sigma_s/\sigma_0 = 4.10^{-2}$, to a loose assembly of particles, with the reference stress $\sigma_0 = k_1/(2\bar{R})$. This desired isotropic stress is slowly applied to the six outer walls. The hydrostatic loading process is considered to be finished when the kinetic energy of the sample is negligible compared to the potential energy. For our sample, the solid volume fraction (volume of the solid particles over total volume) at the end of the hydrostatic loading process is $\nu = 0.676$, which relates to a porosity (volume of fluid and air phases with respect to total volume, in the specific case of asphalt) of $1-\nu = 0.324$.

The second stage of the pressure sintering process is reflected by a *stress relaxation* phase, where the external hydrostatic pressure is strongly reduced, while the adhesion between particles is now made different than zero. Due to the presence of particle contact adhesion, the lateral stability of the specimen remains preserved when the hydrostatic pressure is released, i.e., a coherent and stable particulate structure is obtained that can be subsequently used in the analysis of damage and healing under uni-axial loading conditions. The solid volume fraction of the sample after stress relaxation is decreased to $\nu = 0.63$.

3.2 Response under uni-axial compression and tension

In the uni-axial compression (tension) test, one of the two outer walls, with its normal parallel to the axial (loading) direction, is slowly moved towards (away from) the opposite wall (see Figure 3). The change of the wall displacement in time is prescribed by a cosine function with rather large period in order to limit inertia effects.

The response of the sample under uni-axial compression and uni-axial tension is shown in Figure 4. The normal axial stress σ , normalized by the reference stress σ_0 , is plotted as a function of the normal axial strain ϵ , where positive stress (*strain*) values relate to compression (*contraction*). The stress-strain curves are depicted for different values of k_t (normalized by k_2), which quantifies the adhesion at the particle contacts, see Figure 2. A larger particle contact adhesion increases the effective strength of the sample, both under uni-axial tension and compression. Furthermore, the overall strain at which the effective stress reaches its maximum increases with increasing contact adhesion, k_t .

Note that the maximum stress under uni-axial compression is order of five times larger than under uni-axial tension. A relatively high compressive strength in relation to the tensile strength is typical of various sintered materials, such as ceramics [26], and appears even in asphalt mixtures [15][27]. As further result, from Figure 4, the softening branch under uni-axial tension is somewhat steeper than under uni-axial compression. Here we use a rate that is close to the quasi-static regime, as studied in more detail in [28]. The initial loading branch is linear up to large stress and the initial (elastic) axial stiffnesses σ_t in tension and compression are determined by the sample preparation procedure, and are approximately equal for all the cases considered here, i.e., $\sigma_t/\sigma_0 = 1.04$. The tensile responses are all characterized by local failure at the center of the sample.

3.3 Comparison between numerical simulations and physical experiments

We refer to experiments in [15] to qualitatively compare our numerical investigation with laboratory tests on asphalt mixtures. The authors perform uni-axial unconfined compression tests on compacted samples of dense asphalt concrete (DAC 0/5). The tests are performed in the displacement control mode, at constant axial deformation rates (refer to [15] for details). Mixtures such as DAC are continuously graded (in agreement with our numerical sample) and derive their stability from the packing of the aggregates and the cohesion provided by the bitumen. We report in Figure 4 the stress-strain behavior for the aggregate compressed at different strain rate. Despite the differences between the numerical and laboratory tests, the comparison of Figures 4 and 5 (axial stress versus axial strain on the right side of Figure 5) shows that the elasto-plastic adhesive contact model is able to capture qualitatively the basic features in the behavior of the asphalt mixture, but the strain-rate dependence has to be studied further.

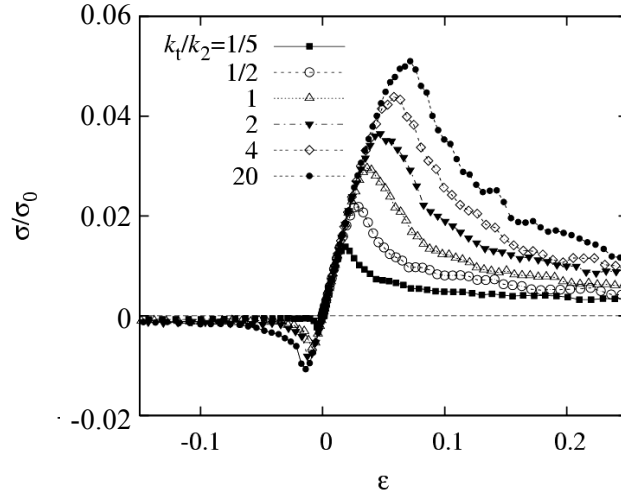


Fig. 4: Dimensionless axial stress (normalized by $\sigma_0 = k_t / (2 \bar{R})$), plotted against axial strain during uni-axial compression (positive stress and strain values) and uni-axial tension (negative stress and strain values), for different particle contact adhesions k_t/k_2 (after [14]).

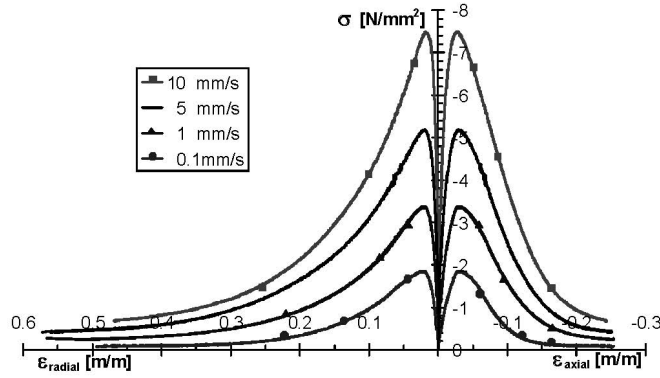


Fig. 5: Axial stress σ versus axial strain ϵ_{axial} and radial strain ϵ_{radial} for uni-axial compression tests on DAC samples at different strain rates and $T=30^\circ\text{C}$ (after [15]). Negative σ means here compression, while negative and positive ϵ mean axial and radial strain, respectively.

3.4 Self-healing under uni-axial compression and tension

In this section we show a possible modeling of induced self-healing mechanisms in asphalt [13]. During uni-axial compression, the sample is stopped at various strains, see Figure 6, and the self-healing is achieved by an instantaneous increase of the particle contact adhesion k_t , which is assumed to be the net-effect of a re-sintering cycle, like warming up an asphalt mixture. Technically, on the contact level, an increase of the contact adhesion k_t corresponds to an increase of the maximum tensile strength $f_{t,max}$, and a decrease of the corresponding displacement $\delta_{t,max}$, i.e. rupture occurs at large tensile strain.

After the application of the re-sintering cycle (self-healing), uni-axial loading is resumed, where the effect of self-healing on the effective stress-strain response of the sample becomes apparent through a comparison of its response with that of both, the unhealed reference sample and a pre-emptively healed sample, which has the stronger contact adhesion from the beginning on.

Under uni-axial compression, see Figure 6(a), or uni-axial tension, see Figure 6(b), the self-healing of the initial sample with $k_t/k_2 = 1/5$ is activated by instantaneously increasing the contact adhesion to $k_t/k_2 = 1$ or 20, uniformly at all particle contacts. Figure 5 shows the response curves after the initiation of self-healing (dashed lines, labeled with the abbreviation ‘SH’), together with the stress-strain responses of the relatively weak ($k_t/k_2 = 1/5$, solid squares), strong ($k_t/k_2 = 1$, triangles) and very strong ($k_t/k_2 = 20$, solid circles) samples. The maximum compressive strength reached after self-healing is larger for healing at smaller deformation – and thus smaller damage. Astonishingly, for all self-healing cases considered, the response eventually converges to the response of the “strong” sample with $k_t/k_2 = 1$ or 20. The strong sample stress-response thus can be interpreted as the response of a pre-emptively “self-healed” sample, where the increase in contact adhesion is initiated at the onset of mechanical loading already. The response of the

sample with $k_t/k_2 = 1$ or 20 acts as envelope for the responses of the self-healed samples with k_t/k_2 increased from 1/5 to 1 or 20, respectively.

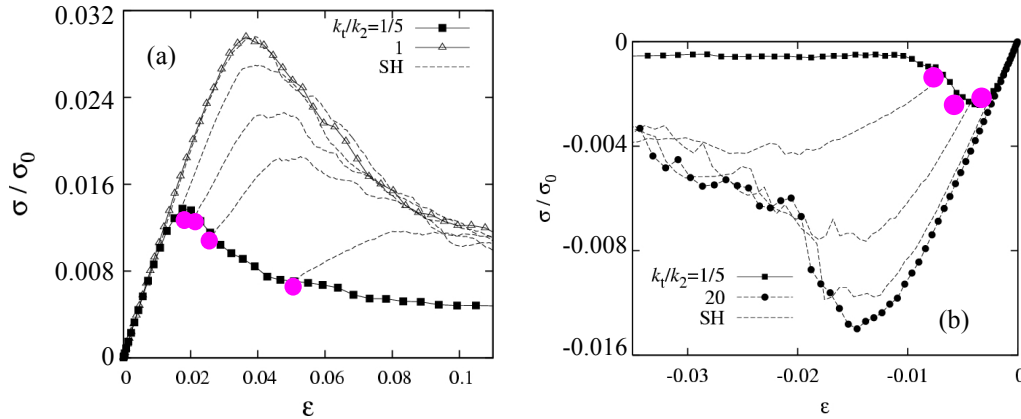


Fig. 6: Axial stress versus axial strain during (a) uni-axial compression and (b) uni-axial tension, for particle contact adhesions $k_t/k_2=1/5$ (solid squares). The initiation of self-healing occurs at axial strains $\epsilon \approx 0.019, 0.022, 0.026,$ and 0.045 for compression and $\epsilon \approx -0.003, -0.005,$ and -0.007 for tension, as indicated by (magenta) dots. The self-healing strength is activated (a) five times and (b) hundred times larger than the original samples' contact adhesion. The self-healing stress responses are given (starting from the different strain points) by the dashed lines. The outer envelope corresponds to self-healing (increase of contact adhesion) already at zero strain (after [14]).

4. MODELING ASPHALT BEHAVIOR AT MACROSCALE

4.1 Simulation of material parameters

When the local behavior has been obtained by DEM analysis, a micro-mechanical based model can be implemented in a Finite Element Analysis code and the macro-scale asphalt response can be reproduced. Using DEM we can simulate element laboratory test (e.g. unconfined uni-axial tests as described in Sections 3.2 and 3.3 or confined uni-axial compression in a Hveem stabilometer [1]) and deduce the basic parameters to model the material behavior.

In this way, the material response during compaction can be reproduced and studied [1]. During compaction of hot asphalt mixtures, particles slide along each other, air is driven out and the matrix becomes denser. An analogy can be established between non-compacted asphalt mixes and wet soils. Critical State theory [29] predicts the soil behavior by using yield loci coupled with specific volume change of the tested material samples, to define plastic deformations. More recently, a model was proposed that involves not only a yield stress, but also the anisotropy of the structure [30][31]. From physical or numerical tests the model parameters, including the growth of the yield locus (related to the applied stress ratio) can be made as a result of densification.

As already mentioned, the numerical element tests represent the bridge between micro-scale (particle-mortar interaction) and meso-scale (multiple particle interaction): during compression, particles move relative to each other, slide and roll because of interparticle friction. Moreover, on the micro-scale one has to take into account how stiff (viscous) the mortar/bitumen layer around the particle is. This parameter also affects sliding of particles and the final local constitutive behavior.

4.2 Modeling the behavior on the macro scale: compaction process

Using the Critical State theory we can go from meso- to macro-scale modeling [1]. Based on the micro and mesoscopic scale information the Critical State parameters for a specific asphalt mixture (and temperature and initial compaction rate) can be estimated. The obtained material parameters can be used for Finite Element Continuum modeling to reproduce, for instance, rolling on asphalt. Then, the horizontal incremental displacement of material can be calculated as a result of a roller pass on a relative non-compacted layer. Fig. 7 shows the results of FE implementation where the constitutive behavior parameters have been obtained from tests with Hveem stabilometer [1]. The simulations indicate that in the upper layer, the material moves in the same direction as rolling, while more in the deeper layer, the material moves opposite to the rolling direction.

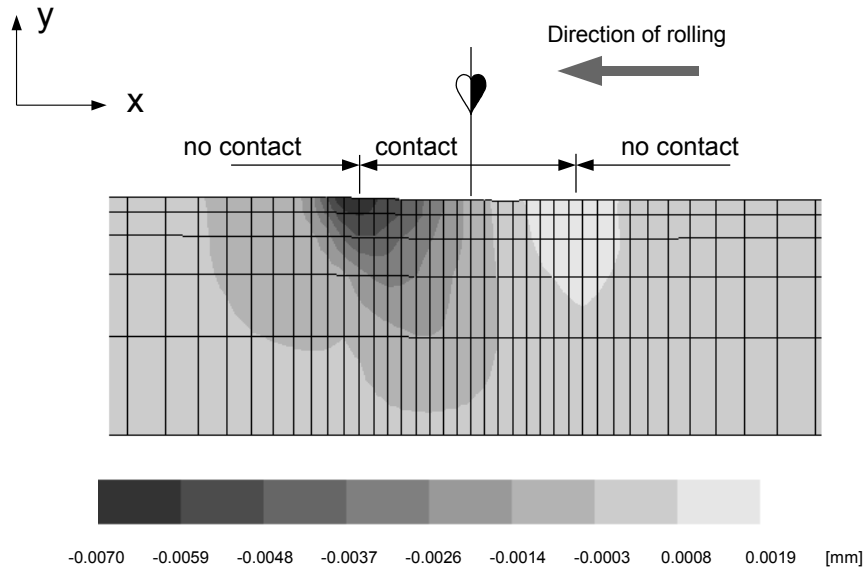


Fig. 7: Incremental material displacements in the x direction, i.e. horizontal material movement. A negative sign means movement in the rolling direction; a positive sign means movement opposite to the rolling direction.

4. CONCLUSIONS

In this work, (1) isotropic preparation, (2) uni-axial deformation, and (3) self-healing processes in damaged adhesive granular assemblies have been studied using DEM simulations with the final goal of application to asphalt mixtures. The effect of self-healing is mimicked by a (global) sintering process, as modeled by increasing the particle contact adhesion from relatively “weak” to rather “strong”.

After isotropic compression, uni-axial compression/tension was applied to the sample for different contact adhesion strengths. While the initial stiffness (slope of the stress-strain curves) is not much affected, the peak strength of the material is: the stronger the contact adhesion, the larger the peak strength. For compression, the strength appears about a factor of five larger than for tension and the softening branch is rather smooth for compression, while the tensile regime shows a sharper drop, resembling more brittle-like behavior.

Moreover, at different strains, the uni-axial deformation is stopped and global self-healing is applied. The stress-strain response obtained from such self-healed samples eventually converges to the envelope curve that represents the damage response of a sample that has the “strong” contact adhesion since the onset of loading. Another result is that the maximum sample strength reached after self-healing very much depends on the deformation level at which self-healing is activated.

Furthermore we show an example of a FE macro-scale simulation of a compaction process of an asphalt mixture used for road pavements. It concerns the simulation of a roller pass on just freshly paved and pre-compacted asphalt. It makes clear that, during a roller pass, while at the top of the layer material moves in the direction of rolling, deeper inside the layer the material moves into the opposite direction. Using such a model requires fundamental correct material parameters. We propose to gain those parameters from the micro- and meso-scale studies with DEM analysis. The model then will be able to indicate how much plastic deformation (material compaction increase) is achieved per roller pass.

This preliminary work shows how powerful DEM simulations can be in describing the constitutive behavior of asphalt mixtures. In fact, discrete simulations give insights on the material microstructure and link observable (macroscopic) phenomena with the kinematics of the interacting components. Very useful information can be extracted from such microscopic analysis, e.g. on how and when to induce self-healing in a damaged material. Finally, given proper parameters from DEM simulations of element tests, a specific constitutive behavior can be implemented in a FE code to describe macro-scale process like rolling compaction.

Future work concerns an interesting investigation issue. The easy switching between adhesive and non-adhesive contact forces in our numerical simulations allows us to separately investigate the role of the single components in the asphalt mixture, focusing in particular on the aggregate skeleton. Through our tool, we want to study how differences in dimension and arrangement of the aggregate skeleton affect the behavior of the full mixture [27][30].

REFERENCES

- [1] Simulation of HMA compaction by using FEM, ter Huerne H. L., van Maarseveen M. F. A. M., Molenaar A. A. A., and van de Ven M. F. C., *Int. J. Pavement Engineering* 9:3,153-163, 2008.
- [2] Review of advances in micro-mechanical modeling of aggregate–aggregate interactions in asphalt mixtures, You Z., Dai Q., *Canadian Journal of Civil Engineering*, 34, 239-252, 2007.

- [3] A discrete numerical model for granular assemblies, Cundall P.A. and Strack O.D.L., *Geotechnique*, 29,47–65, 1979.
- [4] Micro-mechanical modeling for behavior of cementitious granular materials, Zhong X and Chang C.S., *ASCE Journal of Engineering Mechanics*, 125:11, 1280-1285, 1999.
- [5] Micro-mechanical modeling of asphalt concrete in connection with pavement rutting problems, Rothenburg, L., Bogobowicz, A., Haas, R., *Proceedings of the 7th International Conference on Asphalt Pavements I*, 230-245, 1992.
- [6] Simulation of the behavior of asphalt concrete using discrete element method, Chang, G.K., Meegoda, N.J., In: *Proc.2nd Int. Conf. Discr. Element Meth.*, MIT, 437–448, 1993.
- [7] A comparison of micro-mechanical modeling of asphalt materials using finite elements and doublet mechanics, Sadd, M.H., Dai, Q. *Mechanics of Materials* 37, 641-662, 2005.
- [8] Discrete element modeling of asphalt concrete: micro-fabric approach, Buttlar, W.G., You, Z., *TRR*, No. 1757, 111–118, 2001.
- [9] A study of failure in cohesive particulate media using the discrete element method, Ullidtz, P., in: *Proc. 80th TRB Meeting*, Washington, DC, 2001.
- [10] Finite-element analysis and experimental study on tensile fatigue behaviour of bitumen–stone adhesion. *Fatigue & Fracture of Engineering Materials and Structures*, Mo L. T., Huurman M., Wu, S. P. Molenaar A. A. A., 30:9, 823-831, 2007.
- [11] Cohesive, frictional powders: contact models for tension, Luding, S., *Granular Matter* 10, 235-246, 2008.
- [12] A discrete model for long time sintering, Luding, S., Manetsberger, K., Muellers, J., *Journal of the Mechanics and Physics of Solids* 53:2, 455-491, 2005.
- [13] An introduction to material design principles: Damage prevention versus damage management. in: *Self Healing Materials. An Alternative Approach to 20 centuries of Materials Science*, Van der Zwaag S., Van der Zwaag ed., Springer, Dordrecht, NL, 1-18, 2007.
- [14] From discrete particles to solids - about sintering and self-healing (Review), Luding S., *Comp. Methods in Mater. Science* 11:1, 53-63, 2011.
- [15] Asphalt Concrete Response (ACRe) – determination, modeling and prediction, Erkens S.M.J.G, Ph.D. thesis – Delft University of Technology, 2002.
- [16] Improvement of mechanical strength of 8 mol % Ytria-stabilized zirconia ceramics by spark-plasma sintering, Takeuchi, T., Kondoh, I., Tamari, N., Balakrishnan, N., Nomura, K., Kageyama, H., Takeda, Y., *Journal of The Electrochemical Society* 149, A455-A461, 2002.
- [17] In situ strength evolution during the sintering of bronze powders, Shoales, G. A., German, R. M., *Metallurgical and Materials Transactions A* 29a, 1257-1263, 1998.
- [18] Micro-macro transition for anisotropic, frictional granular packings, Luding, S., *International Journal of Solids and Structures* 41, 5821-5836, 2004.
- [19] Quasi-static deformation of a soft particle system, Thornton, C., Antony, S. J., *Powder Technology* 109, 179-191, 2000.
- [20] Assessment of mechanical properties of cohesive particulate solids – part 1: particle contact constitutive model, Tomas, J., *Particle Science Technology* 19, 95-110, 2001.
- [21] Role of anisotropy in the elastoplastic response of a polygonal packing, Alonso-Marroquin, F., Luding, S., Herrmann, H. J., and Vardoulakis, I., *Phys. Rev. E* 71, 051304, 2005.
- [22] On the application of a discrete model to the fracture process of cohesive granular materials, D'Addetta, G. A., Kun, F., Ramm, E., *Granular Matter* 4:2, 77-90, 2002.
- [23] Self-healing of damaged particulate materials through sintering, Luding, S., Suiker, A., *Philosophical Magazine* 88: 28-29, 3445-3457, 2008.
- [24] Evolution of swelling pressure of cohesive-frictional, rough and elasto-plastic granulates, in: *Geomechanics and Geotechnics: From Micro to Macro*, Luding, S., and Bauer, E., In: *IS-Shanghai Conference Proceedings*, 11.-12. Oct. 2010, M. Jiang, L. Fang, and M. Bolton (Eds.), CRC Press/Balkema, NL, 495-499, 2010.
- [25] Modeling particulate self-healing materials and application to uni-axial compression, Herbst, O., Luding, S., *Int. J. of Fracture* 154, 87-103, 2008.
- [26] *Ceramic Microstructures, Property Control by Processing*, Lee, W. E., Rainforth, W. M., Chapman and Hall, London, UK, 1995.
- [27] Permanent deformation of asphalt mixes, Muraya P.M., Ph.D. thesis – Delft University of Technology, 2007.
- [28] Modeling particulate self-healing materials and application to uni-axial compression, Herbst, O., Luding, S., *Int. J. of Fracture* 154, 87-103, 2008.
- [29] *Soil Behaviour and Critical State Soil Mechanics*, Muir Wood D., Cambridge University Press, 1990.
- [30] A local constitutive model with anisotropy for various homogeneous 2D biaxial deformation modes, Luding S. and Perdahcioglu S., *CIT (Chemie Ingenieur technic)* 38(5), 672-688, 2011.
- [31] A local constitutive model with anisotropy for ratcheting under 2D biaxial isobaric deformation, Magnanimo V. and Luding, S. *Granular Matter* 13(3), 225-232, 2011.
- [32] On the equation of state near the jamming transition for polydisperse, smooth, elastic spheres, Ogarko V. and Luding S., submitted, 2011.