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DISCRETE NUMERICAL MODELLING OF CAPSULE-ASPHALT MIXTURE SYSTEM FOR SELF-HEALING PURPOSES

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Abstract. Asphalt mixture faces damage due to vehicle speed, repeated loads, and ultraviolet radiation over time, regardless of being a self-healing material. Induced healing mechanisms are necessary to promote autonomous pavement recovery due to adverse in-service conditions, and the capsule-asphalt mixture system incorporating low-viscosity oils (rejuvenators) has shown to be a possible solution in laboratory tests. This study aims to numerically investigate the effect of rejuvenator-modified mastic (activated capsules) on the stiffness properties of asphalt mixtures within the discrete element method. A three-dimensional model previously validated for rejuvenator-modified mastics with different rejuvenator-to-bitumen ratios (0, 2.5, and 10 wt%) is adopted. A generalised Kelvin contact model represents the time-dependent contacts, and its contact parameters define the rejuvenator amount in the mastic phase. The analysis assesses the impact of the modified mastic amount and the rejuvenator-to-bitumen ratio. Results show that the increasing modified mastic content progressively reduces the mixture dynamic modulus. When the total mastic phase has rejuvenator-modified properties, the mixture stiffness modulus significantly reduces, and the phase angle performs differently from the expected (decrease with frequency) at a 10% rejuvenator-to-bitumen ratio due to the excessively softened state, possibly compromising the pavement mechanical performance. For a 0.30 wt% modified mastic ratio case adopting a local effect, the embedded elements do not significantly influence the mixture rheological properties, especially the stiffness modulus, which may be insufficient for self-healing purposes. Nevertheless, the negligible impact on the phase angle highlights the potential of the rejuvenator-modified asphalt mixture across different traffic and temperature conditions.

Keywords: Discrete Element Method, Rejuvenator-modified Mastic, Asphalt Mixtures, Self-healing.

1 INTRODUCTION

Road pavements are a powerful and effective means of transportation adopted for people and goods for thousands of years. Their applied materials, design methodologies, and construction techniques have constantly evolved to ensure the safety of users. Flexible pavements, which consist of surface layers that use asphalt mixture (AM) that comprises mineral aggregates, bitumen, and air voids, are the most commonly used road pavement system, accounting for more than 90% of the paving systems in Europe and the United States [1, 2]. Asphalt mixtures have their behaviour determined by their constituent materials. While coarse aggregates (90% by weight of the asphalt mixture) are essential in the load-carrying mechanism, the asphalt mastic, resulting from the combination of fine aggregates, filler, and bitumen, enables the composite to withstand tensile and shear stresses. Asphalt materials are sensitive to temperature and heavy repeated traffic loads, which induce early deterioration, thus reducing the pavement lifespan. Other factors, such as vehicle speed, excessive axle loads, ultraviolet radiation, and moisture, also contribute to developing microcracks, eventually leading to macro-cracks [3], and consequently, maintenance costs substantially increase.

Asphalt mixture is a self-healing material [3]. Under ideal traffic and temperature conditions, the binder flows and autonomously repairs the pavement surface. However, in-service conditions are challenging, and pavement researchers have developed strategies to improve its natural self-healing properties [4]. The asphalt industry also seeks to address environmental requirements to reduce CO_2 emissions to achieve a more sustainable infrastructure [5]. One technique is the capsule-asphalt mixture system. This method offers advantages such as an autonomous healing process and the recovery of the aged binder [6]. Implementing this strategy can significantly reduce maintenance costs and greenhouse gas emissions by improving the durability of asphalt roads. In the capsule-asphalt mixture approach, capsules incorporate low-viscosity oil to act upon the initial appearance of microcracks. These capsules remain inactive before being activated by deformation or breakage due to external loads, thus releasing the healing material to the surrounding binder, as illustrated in Figure 1. The rejuvenating oil softens the aged binder, allowing it to flow and drain into the microcracks through capillarity [6]. Researchers have proposed and tested different capsules. Al-Mansoori et al. [3] fabricated calcium alginate capsules and evaluated their effect on mixtures under three-point bending tests, suggesting the method shows a higher strength recovery ratio when compared with specimens without ones in the post-damage and rest stages.

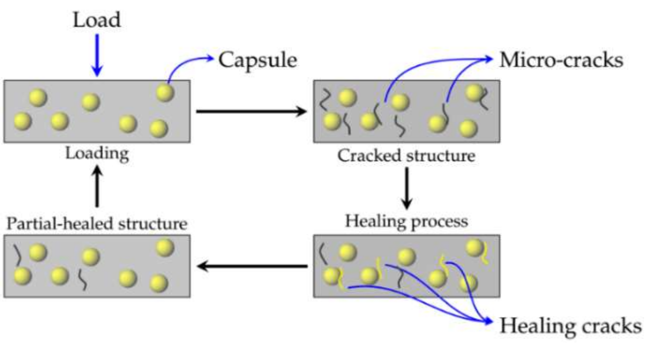

Figure 1. Representation of the crack healing in asphalt mixtures with capsules.

Researchers have adopted three-point and four-point bending tests, indirect tensile tests, semi-circular bend tests, and tension-compression tests to assess the effect of capsules on the stiffness properties of mixtures for representing the loading conditions generated by traffic in asphalt layers [7]. For instance, Norambuena-Contreras [8] concluded that capsule-mixture samples have similar stiffness modulus and higher self-healing properties with respect to neat specimens regardless of the test temperature. However, research mainly focuses on laboratory perspectives, and it is difficult to predict the influence of rejuvenators on other constitutive materials. Numerical simulations should be adopted to acquire meaningful insights. Therefore, this study aims to assess the effect of rejuvenator-modified mastic particles (activated capsules) on the stiffness properties of asphalt mixtures, taking into consideration the number of modified mastic elements and the rejuvenator ratio in the binder. The virtual specimens are subjected to uniaxial tension-compression tests to predict their dynamic modulus ($|E*|$) and phase angle (ϕ) for frequencies varying from 1 to 10 Hz. The time-dependent contacts of the AM specimens adopt a generalised Kelvin (GK) contact model. The modified mastic elements assign distinct GK contact parameters to the contacting particles according to the adopted rejuvenator amount.

2 DISCRETE ELEMENT METHOD

Micromechanical models are adopted to assess the behaviour and properties of asphalt materials under distinct conditions, easing the analysis of recently developed technologies. Numerical models are commonly associated with reducing the need for costly and time-consuming laboratory tests. Recently, pavement researchers have adopted two alternatives for modelling asphalt materials, including the finite element model (FEM) and the discrete element model (DEM). Authors usually utilise the DEM for asphalt mixtures for efficiently modelling large deformation and fracture [9] and apply simple constitutive laws [10]. First introduced for granular materials [11], Rothenburg et al. [12] adopted the method in one of the first asphalt mixture DEM investigations. Over the years, with increasing computational efforts, modelling the behaviour of complex materials, such as asphalt mixtures, has become more accessible and representative. The precision of numerical models has significantly improved with the development of three-dimensional (3D) models and the implementation of more complex contact models to describe the viscoelastic nature of these materials, such as the Burgers model and generalised models.

For instance, Cai et al. [13] assessed the creep behaviour of asphalt mixtures subjected to different stress levels. Al Khateeb et al. [14] numerically modelled the asphalt mixture compaction process, showing that the procedure is thermo-sensitive due to the binder's viscoelastic properties. In addition, Zhang et al. [15] analysed distinct characteristics of aggregates on the permanent deformation of mixtures and mastics at high temperatures, showing that the uniform distribution of aggregates, high friction coefficient, and adequate aggregate angularity positively impact the deformation of mixtures. Other authors have developed methods to optimise contact model parameters. Yi et al. [16] proposed a methodology to calculate and improve the precision of the Burgers contact parameters based on a nano-indentation process and experimental results, suggesting that the simulated results were lower than expected, possibly due to the size of the elements within the specimen.

Recently, numerical studies have assessed the behaviour of capsule-asphalt mixture systems. Zhang et al. [17] evaluated the self-healing capacity of encapsulated asphalt mixtures under different degrees of damage. By implementing two mechanical recovery methods, including radius expansion and particle generation, numerical findings indicated a gradual decrease in the healing capacity of asphalt mixtures as the accumulated damage increased. Câmara et al. [4] investigated the effect of different sunflower oil ratios on the stiffness properties of asphalt mastics under dynamic shear rheometer tests, evidencing that the rejuvenating material progressively reduces the binder viscosity.

3 MICROMECHANICAL MODELLING

3.1 Viscoelastic contact model

Elastic contact models are appropriate to estimate some time-independent properties of asphalt materials, such as stiffness at a specific loading frequency. Several alternative viscoelastic contact models have been developed and implemented within the DEM to consider time-temperature dependency properties. The Burgers contact model gained popularity due to its simplicity [13]. However, complex contact models can improve laboratory test predictions and reduce numerical errors. Hence, this study adopts a generalised Kelvin contact model, previously validated for asphalt mastics and asphalt mixtures [18], to represent the viscoelastic contacts in asphalt mixtures, where its constitutive equations are integrated using a time-centred difference scheme. Figure 2 illustrates the contact model.

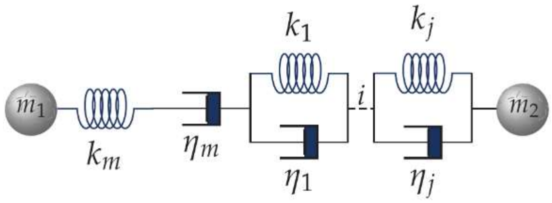

Figure 2. Generalised Kelvin contact model representation.

The model comprises a combination of an elastic portion (κ_m), a viscoplastic portion (η_m), and j-chains of Kelvin elements ($\kappa_{[1-j]}$ and $\eta_{[1-j]}$) placed in series for both the normal and tangential directions. The resulting displacement of the GK contact model derives from the sum of the three components' displacements, while the elements' contact forces are equal. The constitutive equation for the contact force $f^{t+\Delta t}$ of the model is expressed by:

$$f^{t+\Delta t} = \frac{1}{C}\left[u^{t+\Delta t} - u^t + \sum_{i=1}^{j}\left({u_{ve}^{t}}^{i} - \frac{B_i\,{u_{ve}^{t}}^{i}}{A_i}\right)\right] - Df^t \tag{1}$$

where A_i, B_i, C, and D are calculated as follows:

$$A_i = 1 + \frac{\kappa_i \Delta t}{2\eta_i} \qquad\qquad B_i = 1 - \frac{\kappa_i \Delta t}{2\eta_i} \tag{2}$$

$$C = \sum_{i=1}^{j}\left(\frac{\Delta t}{2A_i\eta_i}\right) + \frac{1}{\kappa_m} + \frac{\Delta t}{2\eta_m} \qquad D = \sum_{i=1}^{j}\left(\frac{\Delta t}{2A_i\eta_i}\right) - \frac{1}{\kappa_m} + \frac{\Delta t}{2\eta_m} \tag{3}$$

where Δt is the time step, ${u_{ve}^{t}}^{i}$ is the viscoelastic displacement of the j-chains of Kelvin elements, $u^{t+\Delta t} - u^t$ is the displacement increment, and f^t is the contact force at time t.

3.2 Calibration of viscoelastic contact parameters

The contact parameters for viscoelastic contact models are generally determined based on the fitting of laboratory results of asphalt binders due to the impossibility of defining contact parameters through laboratory tests. A macroscopic GK model is adopted, as shown in Figure 3. This fitting procedure is challenging for generalised contact models because more unknown variables exist.

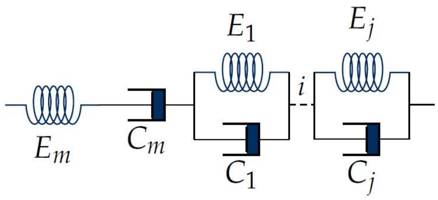

Figure 3. Macroscopic generalised Kelvin model representation.

The response of the macroscopic GK model due to dynamic stress or dynamic strain is defined using the complex modulus, which represents the relationship between stress and strain, which represents the relationship between stress and strain, which are given by:

$$\sigma(t) = \sigma_0 e^{i\omega t}$$
$$\varepsilon(t) = \varepsilon_0 e^{i(\omega t - \phi)} \tag{4}$$

where σ_0 and ε_0 are the stress and strain values at time equals zero, ω is the angular frequency, and t is the elapsed time.

The fitting procedure involves minimising an objective function (F) that captures the relative difference between the model predictions and the laboratory values at each frequency for the dynamic modulus, which can be expressed by:

$$F = \sum_{z=1}^{n}\left[\left(\frac{E'_z}{E'^0_z} - 1\right)^2 + \left(\frac{E''_z}{E''^0_z} - 1\right)^2\right] \tag{5}$$

where E'_z and E''_z are the real and imaginary parts of the predicted dynamic modulus at frequency z, E'^0_z and E''^0_z are the real and imaginary parts of the experimental dynamic modulus at frequency z, and n is the number of data points. It is worth noting that the number of Kelvin elements comprising the generalised model is determined based on an iterative procedure that calculates the error predictions for each study case according to Equation 5.

The set of macroscopic parameters estimated in a previous study [4] to describe the behaviour of asphalt mastics are adopted in the present study to represent the action of the rejuvenating material (sunflower oil) on the stiffness properties of asphalt mixtures. Accordingly, the properties of three rejuvenator-to-bitumen ratios (0, 2.5, and 10 wt.%) are employed, replicating different rejuvenator (oil) amounts in the rejuvenator-modified mastics (oil + mastic) present in asphalt mixtures. These macroscopic properties correspond to the behaviour of three respective mixtures: AM-0 (reference sample), AM-2.5, and AM-10.

In order to convert the macroscopic properties into contact parameters for their use in numerical simulations, the stress-strain relationships of a viscoelastic beam simulating two contacting particles are applied. The contact parameters for the normal direction are given by:

$$\kappa_\xi^n = \frac{E_\xi A}{L}\delta \qquad (6)$$
$$\eta_\xi^n = \frac{C_\xi A}{L}\delta$$

where A is the cross-sectional area of the contacting spheres, L is the sum of neighbouring particles' radii, δ is a coefficient that adjusts the macroscopic properties to the DEM contact parameters, and the subscript ξ assumes i for the Kelvin chains and m for the elastic and viscoplastic units. The parameters for the tangent direction are obtained by the product between the contact stiffness ratio α (κ_s/κ_n) and the values calculated for the normal direction. The estimated values for δ and α for the mastic phase are 1.88 and 0.10, respectively [18].

4 ASPHALT MIXTURE SIMULATION RESULTS

4.1 Virtual specimen generation

This study adopts a three-dimensional asphalt mixture assembly, similar to the one designed in [18]. The virtual sample ($80 \times 50 \times 50$ mm^3) comprises 27646 particles, corresponding to 2739 aggregates and 24907 mastic elements. The mastic phase represents the combination of aggregates with a maximum size of 2 mm and bitumen. A contact network of 160252 interactions associates the particles within the assembly.

Four types of interaction compose the numerical samples. They include the aggregate-to-aggregate, mastic-to-mastic, aggregate-to-mastic, and mastic-to-wall contacts. An elastic contact model and the GK contact model define their behaviours. While the elastic model represents the connections within the aggregate phase and between the mastic and wall elements, the viscoelastic model defines the contacts of the interface phase and within the mastics. The stiffness and the contact stiffness ratio defining the elastic parameters for the aggregate phase, which is considered pure elastic, are 1.20×10^8 kPa and 0.05, respectively, while the parameter α governing the contacts involving mastic particles is 0.10 [18].

Figure 4 illustrates the particle generation process of the non-modified asphalt mixture (reference sample) and the specimen with rejuvenator-modified particles. Aggregate particles (> 2.0 mm) are initially inserted considering a sieve approach, followed by the mastic generation. The rejuvenator-modified particles are then randomly created by converting mastic elements into the desired amount. The numerical simulations investigate the influence of rejuvenator-modified mastic on the mixture rheological response in two different scenarios. In Case 1, the entire set of mastic particles is converted into modified mastic elements and, therefore, adopts rejuvenator-modified properties. This scenario models a lower limit for the asphalt mixtures stiffness properties. In Case 2, 0.30 wt% (by weight of asphalt mixture) of the mastic particles are randomly selected and converted into rejuvenator-modified ones, totalising 235 elements, which is assumed to be an appropriate capsule content for self-healing improving purposes in asphalt mixtures according to experimental analyses [3, 7]. These modified elements have a local effect - only particles in contact with them are affected. Thus, 2355 contacts assume rejuvenator-modified properties. The numerical approach shows a first approximation to the actual asphalt-capsule system once the model directly introduces the activated capsule particles, considering the geometric distribution of these elements within the asphalt mixture specimen.

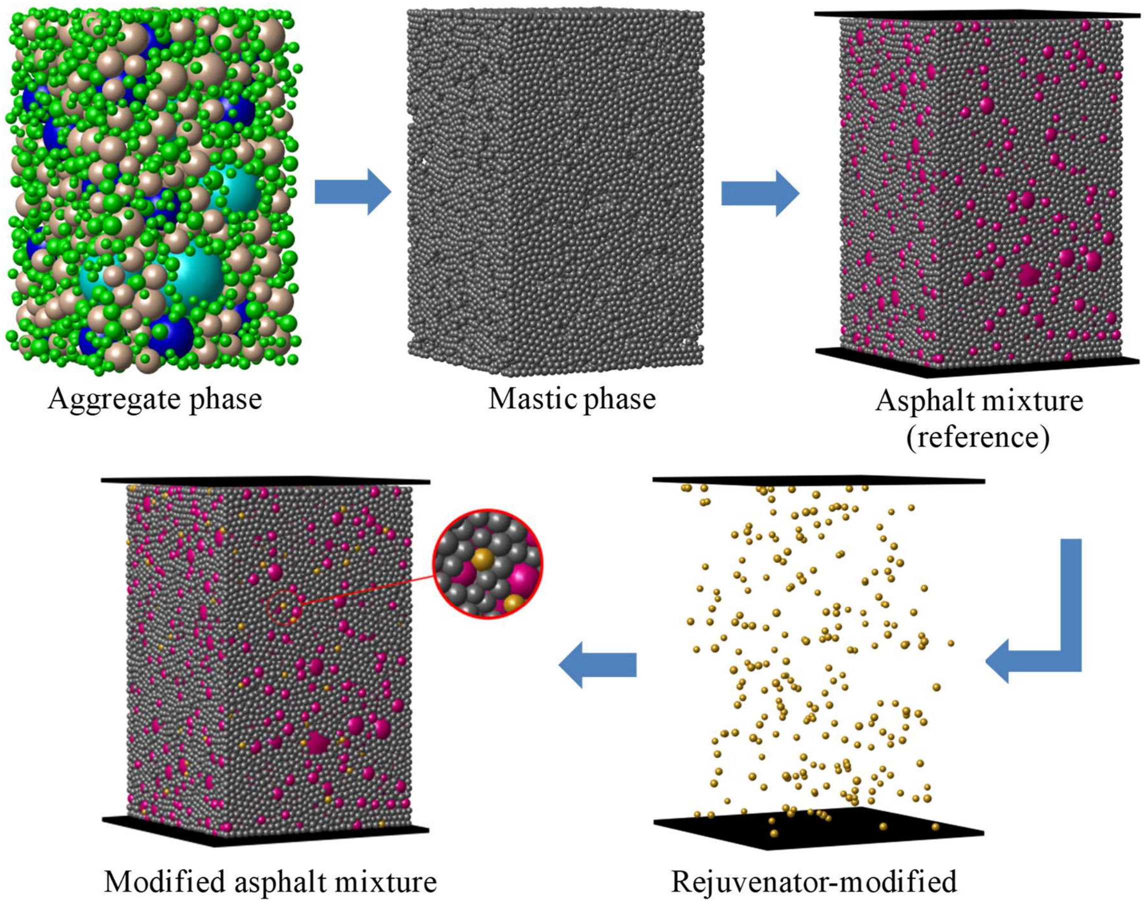

Figure 4. Asphalt mixture numerical generation.

4.2 Numerical test

Asphalt mixture simulations are carried out to validate the numerical study. Uniaxial tension-compression tests are performed on the virtual sample using a strain control mechanism with a magnitude of 1×10^{-4} m/m. Dynamic sinusoidal loads are applied to the particle assembly through the upper wall while the bottom wall remains fixed in all directions. Simulations are conducted at frequencies 1, 2, 5, and 10 Hz for both study cases. The tests continuously monitor the applied strain and resulting stress to calculate the dynamic modulus and phase angle for each loading frequency, as shown in the following equation:

$$|E^*| = \frac{\sigma_{max} - \sigma_{min}}{\varepsilon_{max} - \varepsilon_{min}} \qquad (7)$$
$$\phi = \frac{\Delta t}{T} \times 360$$

where σ_{max} and σ_{min} correspond to the maximum and minimum stress responses, ε_{max} and ε_{min} are the maximum and minimum applied strain values, Δt is the time lag between two adjacent peak stress and strain, and T is the loading period.

4.3 DEM numerical results

The numerical simulation results obtained for both study cases are shown in Figure 5 and Figure *6*. In Case 1 (Figure 5), it is evident that the considerable number of rejuvenator-modified particles significantly reduces the asphalt mixture viscosity, verified by the decrease of the stiffness modulus. This reduction is directly related to the rejuvenator-to-bitumen ratio defining the contact properties of the modified elements, as suggests the evolution of the stiffness modulus on the analysed frequency range, which is expected due to the higher rejuvenator amount representation in the numerical sample. The average stiffness modulus reduction for specimens AM-2.5 and AM-10, at loading frequencies between 1 and 10 Hz, are approximately 42% and 79%, respectively. Despite the possible self-healing heightening benefits, the considerable dynamic modulus reduction observed, especially for sample AM-10, may compromise the pavement mechanical properties.

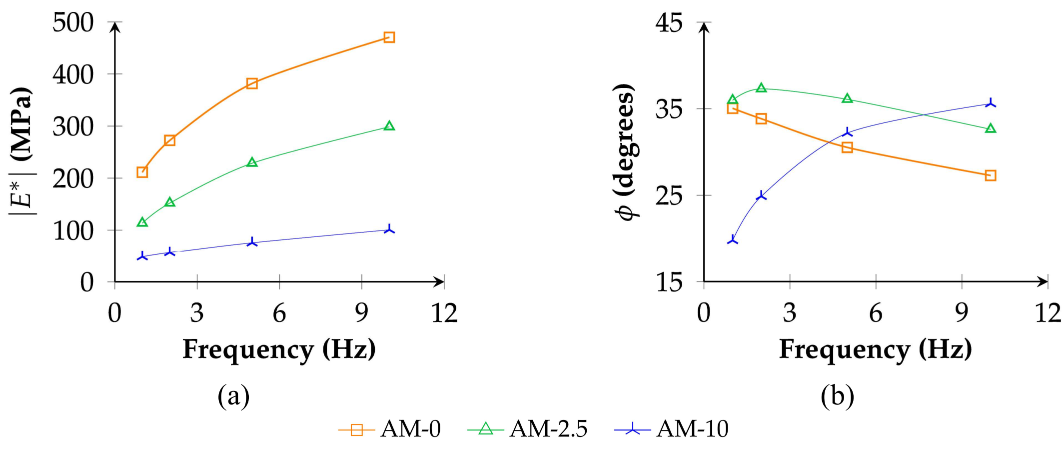

Figure 5. Numerical results for Case 1: (a) stiffness modulus and (b) phase angle.

The phase angle response for the asphalt mixtures also indicates similar effects. For numerical sample AM-2.5, the phase angle slowly increases over the testing frequencies compared with the reference values. Nevertheless, the phase angle development for AM-10 differs from the ones obtained for AM-0 and AM-2.5, particularly for frequencies lower than 5 Hz. This rheological property decreases with the decreasing loading frequency, which is possibly related to the significant amount of rejuvenator-modified mastic that considerably softens the asphalt mixture sample, indicating that the 10% rejuvenator rate defining the viscoelastic contact parameters may be excessive and potentially deteriorates the mixture stiffness properties. This study case indicates that the high number of mastic particles affected by the rejuvenator presented in Case 1 significantly changes the asphalt mixture rheological behaviour, and an appropriate capsule amount should be adopted. Many authors suggest that a maximum capsule rate of 0.50 wt% (by weight of asphalt mixture) is suitable to be adopted for self-healing purposes [19, 20]. In both experimental studies, the 0.50 wt% capsule content increased the healing levels of mixtures and partially restored the properties of aged binder.

Figure 6 shows the numerical results obtained for Case 2. In this analysis, the influence of the activated capsules on the asphalt mixture stiffness properties is slight, considering both rejuvenator-to-bitumen ratios (2.5 and 10 wt%). In the dynamic modulus, for example, the average difference regarding the results for the control sample is lower than 0.50% over the loading frequencies. For the phase angle, the difference varied from -0.02º to 0.20º. The results indicate that a 0.30 wt% capsule representative portion does not significantly influence the stiffness properties of the mixture for both rejuvenator-to-bitumen ratios. The subtle difference in the phase angle also suggests that the asphalt mixture may have acceptable performance on the pavement under different loading conditions.

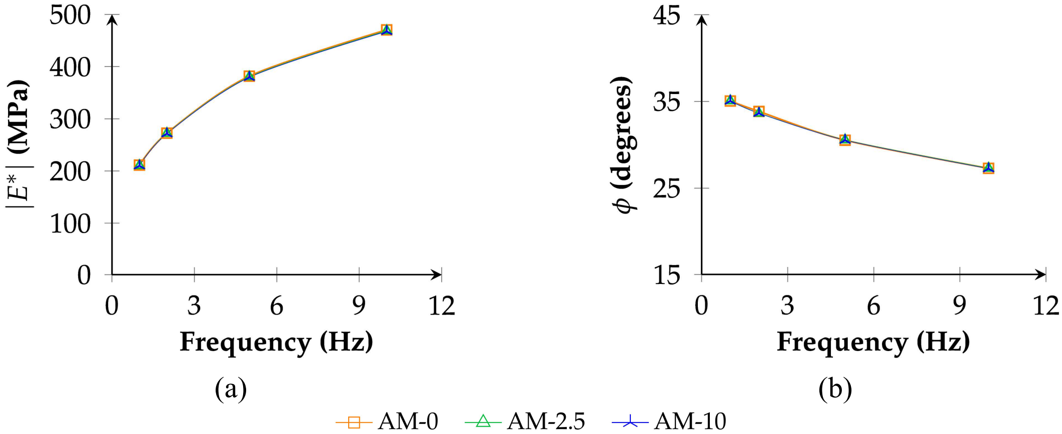

Figure 6. Numerical results for Case 2: (a) stiffness modulus and (b) phase angle.

These effects follow experimental reports. After analysing the rheological behaviour of mastics extracted from asphalt mixtures containing different quantities of capsules, Norambuena-Contreras et al. [21] suggested that a slightly higher capsule amount (0.50 wt%) is sufficient to promote mechanical and self-healing properties of mixtures without significant impacts on their rheological properties. The reduced influence on the rheological properties of mixtures also agrees with the results indicated by Micaelo et al. [7]. Norambuena-Contreras et al. [8] registered a variation of less than 2% in the stiffness modulus of mixtures with a similar capsule ratio in experimental investigations. The less variation for both rheological properties generated in the numerical simulations is possibly due to the different test types, capsule representation, and rejuvenator released during the manufacture of asphalt mixture samples.

The numerical model shows that capsules containing rejuvenators reduce the stiffness of the asphalt mixture to some extent with a proper capsule ratio. Increasing its effect on the mastic particles does not necessarily enhance the performance of asphalt mixtures, and controlling the number of capsules within the specimen should be considered. In order to achieve a higher reduction of the stiffness modulus without affecting the phase angle, numerical simulations should adopt a higher number of rejuvenator-modified elements.

5 CONCLUSIONS

The present study adopts a generalised Kelvin contact model to numerically investigate the effect of the rejuvenator agent (sunflower oil) on the stiffness properties of asphalt mixtures through uniaxial tension-compression tests. The following conclusions were obtained based on the numerical results:

- The asphalt mixture stiffness modulus reduces between 42% and 79% when rejuvenator-modified contacts are adopted in the entire mastic phase, compromising the mechanical performance of asphalt mixtures. Besides, as a consequence of the extended viscous state of the binder, the phase angle acts differently from the expected in most analyses.
- The rejuvenator-to-bitumen ratio defining the contact properties for the modified elements influences the stiffness properties of asphalt mixtures, more evident for specimens with a higher number of modified contacts. The increase in the rejuvenator-to-bitumen ratio indicates the presence of a higher rejuvenator amount in the binder, which leads to a reduction in the asphalt mixture viscosity.
- Simulation results for asphalt mixtures adopting a 0.30 wt% capsule content withs a local effect are close to the results obtained for specimens without modified elements. The impact on the phase angle is very slight, contributing to pavement applications under different loading conditions.

The numerical model was shown to be a suitable approach to model asphalt mixtures with healing agents for considering the spatial distribution of the capsule elements within the specimen. DEM simulations considering the capillary flow (especially when microcracks are present) and the diffusion mechanisms that contribute to reducing the binder's viscosity to highlight the influence of rejuvenators are ongoing.

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