



A micromechanical model to evaluate the impact of air void content and connectivity in the oxidation of asphalt mixtures



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HIGHLIGHTS

- This paper presents a FE micromechanical model of oxidation in asphalt mixtures.
- The impact of the void phase on oxidative hardening of mixtures is evaluated.
- The model includes oxygen diffusion, chemical kinetics and mechanical simulations.
- Dynamic modulus was numerically computed in the first 5 years of pavement service.
- Air void content and connectivity strongly impact oxidative hardening in pavements.

ARTICLE INFO

Article history:

Received 11 December 2013
Received in revised form 24 February 2014
Accepted 9 March 2014
Available online 28 March 2014

Keywords:

Asphalt mixtures
Oxidation
Micromechanical model
Air voids

ABSTRACT

Asphalt oxidation is a chemical reaction between asphalt binders and oxygen that causes irreversible changes in the properties of asphalt materials used in pavement structures. This paper explores the influence of the air void phase of asphalt mixtures on oxidation. Microstructures of an asphalt mixture with probable internal air void structures were generated and implemented in finite elements, and they were used in combination with oxygen diffusion and chemical kinetics models to estimate the changes generated in the mechanical properties of the material. The results confirm that the air void phase strongly impacts the stiffening processes caused by oxidation in asphalt mixtures.

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1. Introduction

An asphalt mixture is a composite material that comprises asphalt binder, air voids and aggregates. During the service life of pavements, asphalt mixtures are subjected to traffic loading and environmental conditions (i.e., temperature, humidity, air contact) that progressively deteriorate the structural capabilities of the material. Within this context, asphalt oxidation is recognized as one of the most important environmental factors affecting the durability of asphalt mixtures.

Asphalt oxidation is defined as the chemical process by which oxygen is added to the polar aromatic compounds of the original

binder [1]. The result of this irreversible reaction is the generation of carbonyl groups and, in a smaller scale, other chemical products including sulfoxide groups. Since carbonyls have higher polarity than the original compounds, the binder becomes stiffer [2]. This rise in stiffness is commonly known as *oxidative hardening*. The rate and magnitude of asphalt oxidation depend on the chemical properties of the asphalt binder, the amount and availability of oxygen sources and other external conditions (e.g., temperature, pressure, etc.) [3].

The scientific literature contains a significant amount of works on the chemistry of asphalt oxidation. Petersen [4] presents a comprehensive compendium of many of these research works. The initial studies on this topic focused on understanding the chemical reactions occurring between oxygen and asphalt binder [5,6], and on quantifying the effect of oxidation on certain physical properties of the binder [7–9]. Plancher et al. [7], for example, measured the changes in both asphaltene content and viscosity during the oxidation of four asphalt binders. The results showed that the

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asphaltene fraction is a dominant component controlling viscosity, and that the raise in viscosity observed in oxidized binders is mainly caused by the increase of this chemical fraction.

Other chemical studies have focused on formulating models of oxidation kinetics [3,10–12]. Petersen [10], for example, conducted a comprehensive study to quantify oxidation rates in terms of the amount of ketons, sulfoxides, and other chemical products. Also, Liu et al. [3] proposed an Arrhenius chemical kinetics model to describe the rate of oxidation as a function of the rate of carbonyl formation. This model was later complemented by Domke et al. [11], who described an initial stage of the oxidation process characterized by a faster rate of carbonyl formation that had not been included in the model of Liu et al. [3].

Even though pavement engineers recognize the role of asphalt oxidation in the performance of pavement structures, the number of works dealing with the impact of this process on the mechanical properties of asphalt mixtures is limited. Several studies have evaluated the change caused by oxidation on the rheological properties of recovered binders from field cores of in-service pavements [13–15]. In terms of asphalt mixtures, Mirza and Witczak [16] developed an empirical model that uses the individual properties of the asphalt binder and the mixture as input data to predict oxidative aging in pavements. Finally, in terms of micromechanical modeling, Sadd et al. [17] developed a finite element model and included damage mechanics to predict the inelastic behavior of asphalt mixtures subjected to oxidation and, more recently, Abu Al-Rub et al. [18] proposed an oxidative aging model that incorporated an internal state variable as part of a continuum damage non-linear viscoelastoplastic model that aimed to predict long-term aging effects in asphalt mixtures.

The current state of knowledge on this topic shows that although the chemistry of asphalt oxidation has been well characterized, there is still limited information explaining the mechanisms of oxidation in asphalt mixtures. Thus, the main objective of this work is to formulate a micromechanical model of asphalt mixtures to evaluate the impact of the air void phase on the evolution of mechanical properties produced by asphalt oxidation. The air void structure was selected as the phase to be studied because it strongly determines the availability of oxygen in compacted asphalt courses and, consequently, it influences the magnitude and extension of oxidation in pavement structures [19,20].

The proposed micromechanical model uses an existing oxidation chemical kinetics model in combination with a finite-element formulation to simulate oxygen diffusion and carbonyl formation, and to characterize the impact of these processes on the macromechanical response of asphalt mixtures over time. As part of the modeling plan, a total of sixty different micromechanical models were randomly created to capture the variability and complexity of the air void phase (i.e., different air void sizes, distribution and connectivity).

The main contribution of this work is that it provides a comprehensive framework to quantify the expected magnitude and uncertainty of the impact of the air void phase on oxidative hardening processes occurring in asphalt mixtures. This information is useful to estimate the actual influence of asphalt oxidation on the durability of road infrastructure projects. Therefore, the results from these modeling simulations could be used, among other possibilities, to plan surface treatment activities required to control or mitigate oxidative hardening in asphalt courses as part of pavement management strategies, or to support the development of compaction quality specifications (e.g., estimate the level of compaction quality required to assure reliable levels of functionality and durability of pavement structures).

The initial part of this paper presents the methodology used in the generation of the micromechanical model. Next, the model and its components are presented, followed by the numerical results.

To conclude, the final section summarizes the most important findings obtained from this work.

2. Modeling methodology

The modeling methodology consisted of six main stages:

1. The geometry of the microstructure of a dense-graded asphalt mixture was generated based on a two-dimensional image of an actual mixture that was obtained using a high-resolution digital camera. This geometry is assumed to represent a fraction of an asphalt mixture located at the top course of a flexible pavement. Similar to other models reported in the literature [21], the micromechanical model contains three main phases: (1) coarse aggregates, (2) a fine aggregate mixture (FAM) which represents the fine matrix of the mixture, and (3) air voids. The first two phases were extracted directly from the image and implemented in the commercial finite element (FE) software Abaqus[®], while the third phase was included in the model as explained next.
2. The air void phase was incorporated into the microstructure following probabilistic principles. The size and amount of air voids were randomly generated, and a specific level of connectivity was assigned to the void structure (i.e., 5% or 10%). Besides, air voids were included into the model following a vertical spatial distribution similar to that observed in actual field cores [22].
3. An oxygen diffusion process was simulated within the microstructure of the mixture, after imposing a boundary condition of 9.28 mol O₂/m² oxygen concentration (i.e., contact of the surface of the pavement with the oxygen present in the air at sea level) to the top of the model and to all connected air voids.
4. Information of diffused oxygen resulting from the previous stage was used in conjunction with a chemical kinetics model to determine the carbonyl area that is being created at every element within the FAM phase through time.
5. The amount of carbonyl area generated at the end of the first, second, third, fourth and fifth year of service (Stage 4) was used to assign different linear viscoelastic material properties to each location within the FAM phase.
6. Cyclic mechanical loading was applied to the top area of the mixture at the end of each year during the first 5 years of service to characterize the impact of oxidation on the overall mechanical response of the mixture through time (i.e., computationally measured dynamic modulus).
7. Steps 2–6 were repeated 60 times, in order to capture the impact of randomness of the air voids phase.
8. The impact of air void content and connectivity on oxidative hardening was analyzed.

In summary, given a specific internal air void structure, the model initially simulates oxygen diffusion within the asphalt mixture. Then, it uses the amount of diffused oxygen and the selected chemical kinetics model to determine the carbonyl area that is generated through time at each location within the FAM phase. This information is then employed to modify the material properties in the FAM phase, and to evaluate the effect of those changes on the overall mechanical response of the mixture through time.

3. Components of the model

3.1. Geometry

As mentioned previously, this work assumes that the microstructure of the asphalt mixture is composed by three constitutive phases: (1) coarse aggregate, (2) FAM, and (3) air

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