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Nonlinear modeling and computational homogenization of asphalt concrete on the basis of XRCT scans

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HIGHLIGHTS

- We study effective mechanical properties of asphalt concrete.
- We propose a novel algorithm for asphalt concrete microstructure generation.
- We analyze X-ray Computed Tomography (XRCT) data.
- We discuss morphological and material nonlinearities.

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ABSTRACT

This paper provides a methodological framework to investigate the effective mechanical properties of asphalt concrete. We, therefore, use numerical tools based on morphological X-ray Computed Tomography (XRCT) data from asphalt concrete specimens. Asphalt concrete is a multi-component material with spatially varying constituents, but in contrast to many other microstructures used in materials science, the partial microscopic material bulk properties of the constituents of asphalt concrete are accessible by physical testing and, therefore, can be considered as well investigated and known. The information gained by the XRCT is used to create artificial Statistical Volume Elements (SVEs) for our numerical investigations. We apply a discrete particle simulation to generate a densely packed sphere model with a pre-defined particle size distribution (PSD) as a first representation of the mineral filler particles. This model serves as the starting point for a weighted Voronoi diagram. Finally, the volume fractions are adjusted by a stochastic shrinkage process of the Voronoi cells. The artificial microstructures are, a priori, generated in a periodic manner and, therefore, possible boundary layer effects during computational homogenization are minimized. The SVEs are considered to be statistically similar to the real structure and serve as its best possible representation. Besides the SVE generation, this paper focuses on the constitutive description of the bituminous binding agent, which we interpret as a viscoelastic fluid. In our analysis of the results we concentrate on the upscaling properties of morphological and material nonlinearities.

1. Introduction

Asphalt concrete is a complex multi-component material widely used for road construction purposes. Its overall mechanical behavior strongly depends on the particular constituents, their individual behavior and their spatial distribution. The typical asphalt compound consists of three major constituents, namely stiff mineral aggregates, a soft viscoelastic binding agent and air-voids [16,40]. Depending on the volume fractions of the constituents, the type of particular constituents and the binding agent, material properties for a wide range of applications can be adjusted in a heuristic manner. Moreover, asphalt concrete represents a multi-scale material, see Fig. 1. From the observer's point of view (length scale L), asphalt concrete can be described as a homogeneous medium with effective material properties. Zooming in, we arrive at the heterogeneous micro-scale (length-scale l) consisting of mineral aggregates, mastic and, possibly, pores. The mastic itself may represent a mixture of the Bitumen phase and very small aggregates $d_{eq} \leqslant 63$ µm. Typically, morphologies with particle sizes 1 mm $\leqslant d_{eq} \leqslant$ 8 mm can be reliably resolved by the X-ray Computed Tomography (XRCT) technique with resolution on the micrometer-level. Hereby, the PSD is expressed in terms of the diameter of volume equivalent spheres

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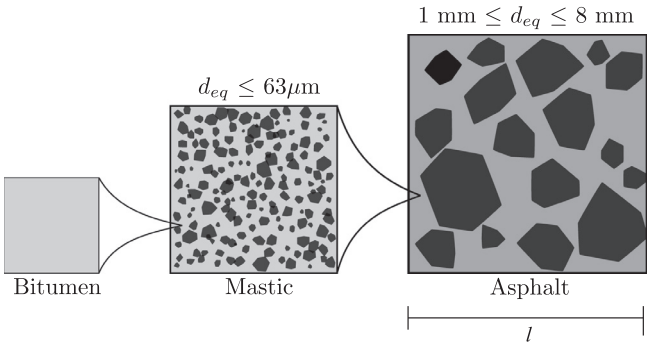

Fig. 1. Different scales for asphalt concrete.

$$d_{\mathrm{eq}} = \sqrt[3]{\frac{6\,V_{3D}}{\pi}}, \tag{1}$$

with the particle volume V_{3D} extracted from the XRCT data.

It is an ongoing research field to understand the highly complex interactions between the microscopic processes and the prevalent material properties of asphalt concrete on the large scale for these strongly heterogeneous materials. Hence, numerical modeling approaches are valuable tools for this analysis.

In order to describe the microscopic processes under external loading, detailed information about, first, the material properties of the microscopic constituents and, second, about the morphology of the composite for a SVE that is the spatial arrangement of the constituents, is required. Hereby, the morphology of the mineral aggregates that is, amongst others, their volume fraction, the grading curve as well as their particle size distribution (PSD), is of particular interest. Thus, it is necessary to gain knowledge about these properties to create the best possible data basis for numerical simulations. In our study, this morphological knowledge is gained by a physical specimen which is scanned by XRCT. The 3-dim analysis software Avizo Fire (FEI Visualization Sciences Group, Version 9) gives us the opportunity to extract the morphological properties from the reconstructed volume, since some of them are not known from the production process itself. In the upcoming sections, we propose a workflow from the raw XRCT data towards statistically similar unit cells used for the computational homogenization process of the overall material properties of the compound. For this purpose, this paper combines scientific approaches from different disciplines. We, therefore, want to give an overview on the current research in these fields and to review the findings shortly.

Finite element (FE) simulations on data gained from XRCT is a research field investigated by various groups in different areas, such as material sciences and engineering with particular regard to the image acquisition of asphalt concrete and the quantitative analysis of the microstructure to determine phase volumetric relationships and aggregate characteristics. Onifade et al. [28] studied the micro-mechanical results and displayed the load transfer chains and stress localizations between neighboring particles. You et al. [42] investigated a large biphasic example by ignoring air-voids. They introduced the mastic as a thermo-viscoelastic, thermo-viscoplastic and thermo-viscodamage material. The mineral aggregates are modeled as a linear elastic material. Coleri and coworkers carried out a prediction of the asphalt concrete shear modulus [3]. They developed 2- and 3-dim micromechanical FE models with elastic and viscoelastic constitutive behavior for the constituents. Two different asphalt mixtures were investigated with a shear frequency sweep at constant height. They found a very good accuracy for the three dimensional example. Further, they showed an interesting comparison between the virtual image of the mineral aggregates and the real structure.

Since, however, numerical simulations based on XRCT scans using triangulated surfaces are highly expensive in terms of CPU-time and the flexibility for the creation of several different microstructures is not given [42], we now want to focus on literature which is concerned with the creation of artificial microstructures. These artificial microstructures have the advantage that a large amount of microstructures can be created and investigated in a short time frame. Tehrani and coworkers introduced a custom numerical toolbox [39] that is a random object modeler, to generate random inclusions of various sizes and shapes to derive the aggregate skeleton. The asphalt concrete is modeled as a biphasic medium with linear viscoelastic behavior for the bituminous binding agent. Results in terms of complex moduli and phase angles and also localized stress and strain distributions are studied. The calculations are carried out in 2-dim but cut out from 3-dim microstructures. In another work of Tehrani et al. [38], the results for linear viscoelastic simulations in 3-dim with only spherical inclusions are shown. However, geometrical as well as material linearity is a very strong assumption for such heterogeneous media with strongly diverging material properties as the asphalt constituents.

The generation of artificial microstructures using Voronoi tessellations or Voronoi diagrams is a well-established technique for modeling of crystalline structures and reinforced composites [8,9] as well as for concrete models using a random structure of spherical aggregates [10,41]. However, it is not possible to control a PSD by the standard Voronoi tessellation. To remedy this deficiency, Lavergne and coworkers [21] proposed to generate microstructures with pre-defined PSD and grain shapes using dense sphere packing and power diagrams [1,2] for polycrystals. They, therefore, combine the weighted Voronoi tessellations with the simulation of a particle dynamics approach. The used algorithm for the polydisperse sphere packing is the Lubachevsky–Stillinger algorithm [24]. In the present contribution, we extend this approach towards asphalt concrete, where the volume fraction of solid mineral aggregates is significantly smaller than 1, as it is the case for polycrystals. As the basis for our PSD we make use of a XRCT data set.

Besides the morphology on the micro-level it is important to investigate the material properties of the particular constituents with special regard to the bituminous binding agent, generally understood as a viscoelastic material. Concerning the rheological models for the bituminous binding agent, a wide range of research activities are to be found in literature. We would like to refer to the extensive literature review for the mechanical modeling of the linear viscoelastic rheological properties of the bituminous binding agent by Yusoff and coworkers [43] including the master curve procedure and the time–temperature superposition principle [6] that we apply in Section 3. Furthermore, fractional models [37] and nonlinear viscoelastic rheological models [15,31], to name only a few, are to be found in literature. In the present contribution we refer to the generalized Maxwell-Zener approach extended to a 3-dim continuum formulation with consideration of geometrical nonlinearities [14,36].

Having all material properties of the viscoelastic compound on the micro-scale at hand, we derive the macroscopic response of the mixture to an external loading by a computational homogenization approach based on volume averaging techniques. Assuming separation of scales $l \ll L$, we apply Hill's [13] averaging framework based on a two-scale energy balance, the so-called Hill–Mandel principle of macro-homogeneity, to compute the effective material properties in terms of volume averages of their microscopic counterparts. For this purpose, we have to define a microscopic volume element being representative for the entire structure (Representative Volume Element, RVE). For practical applications, the size of