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A framework for 3D synthetic mesoscale models of hot mix asphalt for the finite element method

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HIGHLIGHTS

- An algorithm to create 3D synthetic mesoscale models of hot mix asphalt is presented.
- Particle size distributions are captured by nested Voronoi tessellations.
- The complex shear modulus and loss angle are predicted using the finite element method.
- The representative volume element size is found to increase reciprocally to loading frequency.

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ABSTRACT

A versatile framework to create 3D mesoscale models of hot mix asphalt is presented. The mortar phase of a German standard hot mix asphalt is tested in the linear viscoelastic regime using a modified dynamic shear rheometry setup. The widely used generalised Maxwell-model is fit to master-curve data. Virtually any particle size distribution can be matched by a nested Voronoi tessellation algorithm, which is shown by generating geometrical models for three different types of hot mix asphalt. Several techniques to reduce the computational effort are introduced at the geometry and mesh levels. Representative volume elements for mixture SMA 8 S are determined and used to predict the complex shear modulus and loss angle. An analysis of the reinforcing properties of the mineral aggregate phase is presented. The influence of the loading rate on the size of representative volume elements is investigated.

1. Introduction

Asphalt is a composite material consisting of bituminous binders, mineral aggregate, and voids. Its intricate mechanical behaviour features strong thermal, time, and rate dependencies, just to name a few. These properties depend mainly on the properties of the bituminous binders used in asphalt. However, real and virtual experiments have shown ubiquitously, that the representative sample size depends mainly on geometric factors like volume fraction and nominal maximum aggregate size (NMAS) [49]. Furthermore, the material contrast between the constituents is known to influence the variability of mechanical response and therefore representativeness, see e.g. [46,60]. The understanding of the mechanical properties of composite materials usually requires a geometric model of the underlying structure and mechanical models of the resolved constituents at appropriate scales. Combined, these separate models represent the material at a larger scale. Furthermore, predictive modelling also asks for high flexibility, such that the combined model can guide research and development. The present work focuses on the extension of a previous model [60] to more realistic constitutive and geometric modelling.

Any mesoscale model of asphalt has to define a size threshold for the geometrical entities it resolves. Below this threshold, a continuous mortar[2] phase is assumed, which consists of bitumen and aggregates smaller than the threshold, see Fig. 1 for an illustration of the scale separation used here. A threshold of 2 mm is a natural choice for particle size distributions (PSDs) based on the metric system [3,17,28,61]. The cumulative mass percentage of passing aggregates at this sieve size is always given by German standards [2,19]. Consequential, dynamic shear rheometry according to DIN EN 14770 [1] for testing pure bitumen cannot be applied to measure the properties of the viscoelastic mortar phase using standard

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[2] Also termed fine aggregate matrix (FAM) in the corresponding literature.

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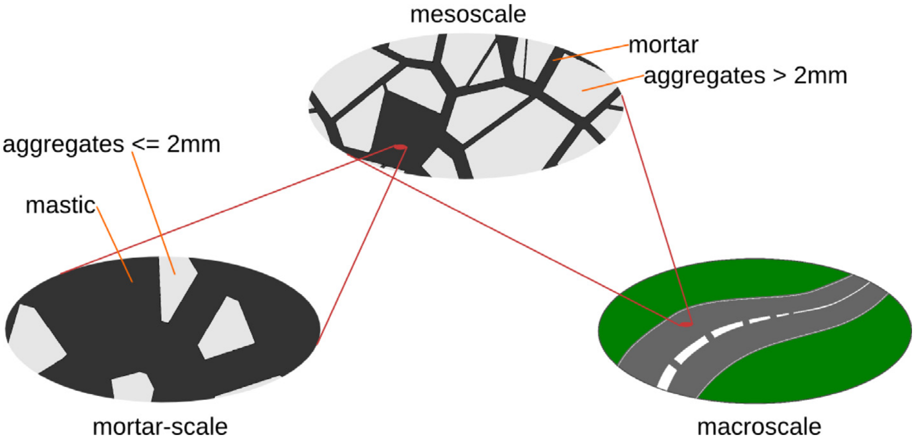

Fig. 1. Scale separation within asphalt used here.

equipment because the required gap widths are too large. Therefore, the rheometer was modified regarding the test specimen dimensions. This modified setup and the calibration of a generalised Maxwell model using master-curve data are presented in Section 2.

Image based modelling has become an indispensable tool to analyse and understand the complex behaviour of asphalt. 2D models can be obtained from simple images, see e.g. the works of Aragão et al. [4], Caro et al. [8], Karki et al. [31], Ozer et al. [46], Wang and Hao [58]. These models require only moderate computational resources, but it has been shown that 2D modelling is often not valid. Fakhari Tehrani et al. [17] concluded that the reduction to two dimensions is only valid in the case of low aggregate volume fractions and high loading frequencies. Several research groups found that a 2D model underestimates the stresses w.r.t. a 3D model [9,10,40,46]. 3D models typically rely on XRCT scanned samples, see e.g. the works of Coleri et al. [10], Kutay et al. [35], Schüler et al. [54], You et al. [64]. Image based modelling requires that the geometry, which is to be modelled, has to exist *a priori*. However, it is worthwhile to have a synthetic method at hand which can generate geometries of not yet existing asphalt mixtures. Synthetic 2D geometry generators for asphalt are reported to use circles and ellipses [27,40,53], or polygons [11,32,34,59,70]. A comparison of a 2D synthetic random elliptical inclusions model with an image based approach did not show significant advantages of the image based approach [39]. However, the accuracy of the aggregate shapes is critical, as Yang et al. [63] emphasise in a review article about heterogeneous modelling efforts of stone based materials.

Only a few synthetic 3D geometry generators for the finite element method[3] have been reported. Mo et al. [40] developed a monodisperse sphere model for ravelling analysis of porous asphalt. Dai [12] also used a monodisperse sphere model with damage modelling to compute indirect tension and compression experiments on virtual samples. Fakhari Tehrani et al. [17] proposed a spherical inclusion model for mastic and mortar. In a previous publication, they also showed a 3D polyhedral geometry, but computations were executed on 2D slices [18]. A similar path is followed by Cao et al. [7], who used a 3D compaction simulation but moduli predictions were executed in 2D. Chen et al. [9] used extruded polygons, which are not strictly convex. They presented parameter studies of aggregate orientation as well as air void distribution and size. Schüler et al. [54] used a discrete particle simulation to create a weighted Voronoi tessellation (VT) which represents the PSD of a German standard open-porous asphalt. They employ their method to simplify the geometry of an XRCT scanned sample, but the approach could be used in a completely synthetic manner. In this contribution, a different method is pursued which creates an initially monodisperse random[4] VT and then iteratively retessellates (thus nested tessellation) aggregates until the desired PSD is matched. This method creates clusters of fine aggregates, which are typically encountered in real asphalt types.

As it is widely known that VTs are badly conditioned for meshing, ideas to improve the geometry have been around for a while, see e.g. Nygårds and Gudmundson [43]. Nevertheless, regularisation of VTs is not frequently undertaken. Here, the nested tessellation uses Voronoi cells to cut Voronoi cells, resulting in a high amount of disadvantageous features like small interior angles, tiny facets, and short edges. Thus, a regularisation method based on a naive heuristic is used which removes small triangles. The microstructural modelling is presented in Section 3.

Among the boundary conditions that satisfy the Hill-Mandel condition, periodic displacement boundary conditions are the preferred choice in order to establish minimally sized representative volume elements (RVEs). The response under displacement based periodic boundary conditions is known to be bounded by linear displacement and constant traction boundary conditions from above and below, respectively, see e.g. Hori and Nemat-Nasser [24], Huet [25], Miehe [38], Ostoja-Starzewski [45], Saeb et al. [50]. Based on these theoretical findings, several authors predicted the macroscale response of viscoelastic composites using computational homogenisation, see e.g. Schüler et al. [53,54], Zhang and Ostoja-Starzewski [66,67]. Periodic boundary conditions require periodicity of geometry and mesh at the domain boundary. Periodic random VTs are generated using seed periodisation, see e.g. Decker and Jeulin [13], Fritzen and Böhlke [20], Wimmer et al. [60]. This technique extends to nested VTs.

Typically, the convergence of the local fields in RVEs requires a high mesh density, while representativeness asks for large sample volumes. Thus, computational resources are easily exhausted, which forces researchers to reduce their statistical requirements, see e.g. Schüler et al. [54]. In order to reduce the computational complexity, an inhomogeneous mesh density is used in the present contribution which required additional attention to obtain periodicity. An overview of finite element based modelling including boundary conditions and meshing is given in Section 4.

Numerical results of the homogenised mechanical properties of German standard type stone mastic asphalt (SMA 8 S) are presented

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[3] Generators for the discrete element method are not considered here.

[4] The peculiarities of pseudorandom number generation are out of scope of this paper. Hence "pseudo" is dropped for reasons of brevity.