
Mesomechanical Modelling of Asphalt

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Overarching Abstract

Asphalt is one of the oldest construction materials known to mankind. Unfortunately, it is also one of the most complex materials. Asphalt exhibits elastic, viscous and plastic properties. Furthermore, it damages and shows significant ageing over the course of a few decades. These properties are inherited mostly from the bituminous binder. However, asphalt is actually a random heterogeneous material consisting of mineral aggregate glued together with bitumen. Mixed together, asphalt acquires all the properties of a true composite material: stiffening and strengthening, localisation, scale dependency, and many more.

The present work deals with the modelling of asphalt used in road construction. Due to its complexity, asphalt is difficult to model as a bulk material on the macroscale. The rationale is to develop a mesoscale model of asphalt within a computational mechanics multiscale framework. The mechanical field equations are solved using the finite element method. Here, asphalt is separated into two components, namely asphalt mortar and coarse aggregate. This divide and conquer approach leads to simpler submodels, and has the additional benefit of modularity.

This cumulative thesis starts off with background information about the history of asphalt, its constituents, mechanical properties and design (section 1).

Following the idea of modularity, the first publication (section 2) establishes the multiscale framework in general. A first method to generate geometries of random heterogeneous angular particle systems based on Voronoi tessellation is developed (section 2.3). Tetrahedral finite element meshes are generated (section 2.3.3) and a strain driven first order homogenisation method is employed to compute macroscale material parameters (section 2.5). So far, material modelling resorts to linear elasticity (section 2.4).

The second publication (section 3) is specialising almost every aspect of the previous publication w.r.t. road engineering. Material modelling is based on linear viscoelastic data obtained by dynamic shear rheometry. The generalised Maxwell model is used (section 3.3). Geometry generation is extended to represent particle size distributions of several real mixtures (section 3.4). The meshing procedure does now use coarse-graining for volumes where high accuracy is not needed (section 3.5.2). Upscaling from meso- to macroscale is performed in time domain at a temperature of 20 °C and a frequency of 1 Hz (section 3.5). At this stage, validation against experimental mix data becomes possible.

The realm of computational mechanics is somewhat left in the third publication (section 4), which concentrates on the analysis of irregular polyhedra instead. Particular, the ambiguous notion of “size” for non-spherical particles is assessed. The methodology is based on principal component analysis of the inertia tensor using discrete computational geometry. This is used as a basis to propose estimators for sieve size (section 4.3). Several shape descriptors are introduced and compared between data from X-Ray CT scanning (section 4.3.5) and synthetic data (section 4.3.6). With suitable datasets at hand, the quality of sieve size estimation as a function of sphericity is investigated (section 4.5.2 and section 4.5.3).

Additional investigations, which are mostly unpublished yet, are presented in section 5. Unfortunately, some shortcomings have been revealed after publication of the three articles, which are also addressed in this chapter.

Übergreifende Kurzfassung

Asphalt ist einer der ältesten der Menschheit bekannten Werkstoffe, leider aber auch einer der komplexesten. Asphalt weist elastische, viskose und plastische Eigenschaften auf. Weiterhin schädigt er und altert über einen Zeitraum von wenigen Dekaden. Diese Eigenschaften stammen größtenteils vom Bindemittel Bitumen. Jedoch handelt es bei Asphalt um einen zufallsbasierten heterogenen Werkstoff — mit Bitumen verklebte Gesteinskörnung. Gemischt erhält Asphalt alle Eigenschaften eines echten Kompositwerkstoffes: Versteifung und Verstärkung, Lokalisierung, Skalenabhängigkeit, u.v.m.

Die vorliegende Arbeit beschäftigt sich mit der Modellierung von Straßenbauasphalt. Aufgrund seiner Komplexität kann Asphalt nur schlecht im Gesamten auf der Makroskala modelliert werden. Die Grundidee dieser Arbeit ist daher die Entwicklung eines Modells auf der Mesoskala, innerhalb des Rahmens von Multiskalenmethoden der numerischen Mechanik. Die mechanischen Feldgleichungen werden dabei durch die Methode der finiten Elemente gelöst. Asphalt wird gedanklich in zwei Bestandteile zerlegt: Asphaltmörtel und grobe Gesteinskörnung. Dieser “Teile und Herrsche”-Ansatz führt zu einfacher zu handhabenden Teilmodellen, und hat weiterhin den Vorteil eines Baukastenprinzips.

Diese Arbeit beginnt mit Hintergrundinformationen zur Geschichte des Asphalts, seiner Bestandteile, mechanischen Eigenschaften, sowie Mischgutgestaltung (section 1).

Dem Konzept der Modularität folgend wird in der ersten Veröffentlichung das grundlegende Mehrskalenmodell aufgestellt. Eine erste Methode zur Erzeugung kantiger zufallsbasierter heterogener Partikelsysteme durch Voronoi Tesselierung wird entwickelt (section 2.3). Tetraedernetze für die Finite-Elemente-Methode werden erstellt (section 2.3.3) und eine dehnungsgesteuerte Homogenisierungsmethode erster Ordnung wird zur Berechnung von Materialparametern der Makroskala verwendet (section 2.5). Zunächst wird linear elastische Materialmodellierung betrieben (section 2.4).

Die zweite Veröffentlichung (section 3) spezialisiert beinahe jeden vorhergehenden Aspekt mit Bezug auf den Straßenbau. Die Materialmodellierung wird durch das generalisierte Maxwell-Modell linear viskoelastisch und basiert auf Daten, die durch dynamische Scherrheometrie erhoben wurden (section 3.3). Die Geometriegenerierung bildet nun die Korngrößenverteilungen verschiedener echter Mischungen ab (section 3.4). Das Finite Elemente Netz ist an Stellen mit geringen Genauigkeitsanforderungen vergrößert (section 3.5.2). Der Skalenübergang wird im Zeitbereich bei einer Temperatur

von 20 °C und einer Frequenz von 1 Hz durchgeführt (section 3.5). Ab hier ist die Validierung mittels Experimentaldaten von realem Mischgut möglich.

Die dritte Publikation (section 4) beschäftigt sich mit der Analyse unregelmäßiger Polyeder. Insbesondere wird der Begriff “Siebgröße” analysiert, der bei nicht kugelförmigen Partikeln mehrdeutig ist. Die Methodik basiert auf einer Hauptkomponentenanalyse des Trägheitstensors mittels diskreter Computergeometrie. Diese Grundlage wird zur Formulierung von Schätzern für die Siebgröße verwendet (section 4.3). Verschiedene Formkenngrößen werden vorgestellt und für Röntgen-computertomographische (section 4.3.5) und synthetische Daten (section 4.3.6) miteinander verglichen. Mit brauchbaren Datensätzen ausgerüstet wird die Güte der Siebgrößenvorhersage als eine Funktion der Sphärizität untersucht (section 4.5.2 and section 4.5.3).

Zusätzliche Analysen, die größtenteils bislang unveröffentlicht sind, werden in section 5 vorgestellt. Bedauernswerterweise wurden nach Veröffentlichung der drei Artikel einige Inkonsistenzen gefunden, die ebenfalls in diesem Kapitel diskutiert werden.

“Alles Wissen und alles Vermehren unseres Wissens endet nicht mit einem Schlußpunkt,
sondern mit einem Fragezeichen.” — Hermann Hesse

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Acronyms

CPU Central Processing Unit.

DOF Degree of Freedom.

DSR Dynamic Shear Rheometry.

EDE Equivalent Dimension Ellipsoid.

EVb Equivalent Volume Box.

EVE Equivalent Volume Ellipsoid.

EVS Equivalent Volume Sphere.

FAM Fine Aggregate Matrix.

FE Finite Element.

HMA Hot Mix Asphalt.

IAEG Intra-Aggregate Element Growth.

MA Mastic Asphalt (Gussasphalt).

NMAS Nominal Maximum Aggregate Size.

PBC Periodic Boundary Condition.

PMB Polymer Modified Bitumen.

PSD Particle Size Distributions.

PVT Pure Voronoi Tessellation.

RUC Repeating Unit Cell.

RVE Representative Volume Element.

SMA Stone Mastic Asphalt.

SSA Specific Surface Area.

SSD Steady-State Dynamics.

VT Voronoi Tessellation.

VP Voronoi Polyhedr{a,on}.

XRCT X-Ray Compute{d,r} Tomography.

1 Overarching Introduction

The present work deals with computational modelling of asphalt, particularly with meso-scale models of Hot Mix Asphalt (HMA) in roadway engineering. Asphalt is a natural or artificial composite of bitumen and mineral aggregate [13], see figure 1.1 for two modern examples. It is commonly used in road construction for pavements, in building construction for floor coverings, in hydraulic engineering and more rarely in landfill construction for waterproofing [90]. In American English language use, “asphalt” usually refers to what is called “bitumen” outside the United States. There, the word “asphalt” is often used as shorthand for “asphalt concrete“. In order to complicate matters, “asphalt concrete” is the name of a particular type of asphalt with minimal void content [65].

The word asphalt is derived from the Ancient Greek “*ásphaltos*”, which means “not-falling“ [194]. The word concrete comes from the Latin word “*concretus*“, which means cohering or condensed. Bitumen inherits its name from Latin “*pix tumens*“, meaning exuding, or bubbling, pitch. Nevertheless, bitumen must not be confused with pitch, which is distilled from tar, which is in turn derived from coal. Due to its high content of polycyclic aromatic hydrocarbons, pitch is highly cancerogeneous and no longer used in road engineering in Germany¹ and most other European countries [75].

1.1 History

Asphalt is one of the oldest construction materials known to mankind. Bitumen occurs naturally in natural asphalt, such as in the famous La Brea Pitch Lake in Trinidad, Lake Guanoco in Venezuela, the Dead Sea, Val de Travers in Switzerland, and many more locations. Based on archaeological excavations, natural asphalt was already used to produce tools in prehistoric times around 40,000 BC [49]. For building construction, asphalt has been used by the Sumerians between 3200 and 2900 BC. The material was often used in the Mesopotamia region, as natural asphalt deposits were present there [25; 49]. People used it to waterproof containers and reed boats. Furthermore, they used the material as a mortar for adobe bricks. In Egypt, it was used in the mummification process [136]. A hint on its usage can also be found in the Bible in Gen 11,3 in the story of the Tower of Babel, which, according to a strictly biblical chronology, dates back to around 2300–2200 BC.

¹West Germany: 1970, Formerly East Germany: 1990



Figure 1.1: Drill core with two different types of asphalt. The top layer is an open-porous asphalt, whereas the bottom layer is dense. Published under CC-BY-SA-3.0 as "Core porous asphalt" by VBW-Asfalt, cropped from original.

For road construction, asphalt has been used in Babylonian times earlier than King Nebuchadnezzar II reigned (605–562 BC). An inscription on a brick found in Babylon states that Nebuchadnezzar’s father, Nabopolassar, King of Babylon, “had made a road glistening with asphalt and burnt bricks”, and that he, “Nebuchadnezzar, King of Babylon, he who made Esagla and Ezida glorious, placed above the bitumen and burnt bricks, a mighty superstructure of shining dust, made them strong within with bitumen and burnt bricks as a high-lying road” [167].

The Romans, famous for their road-building skills, recognised the importance of load-bearing substructures. Most of the higher quality roads were composed of five layers. Instead of asphalt, they did use lime-based cement (*opus caementicium*) as a binder for their most important roads [53]. Several Roman roads survived for millennia; some are even overlaid by modern roads.

During the middle ages, most of the ancient knowledge became lost. Unknown to western civilisations however, the Incas of Peru constructed some roads which were paved with a composition similar to modern bituminous mixtures around 1500 AD[53].

The first attempts to bring post-Roman science to road building included unbound gravel, cobblestones, bricks, and setts². The latter are still in widespread use on urban roads, particularly for their decorative appearance, but must not be used for heavily loaded roads[10].

In the late 18th to early 19th century, several engineers proposed new concepts for roads, addressing particularly issues with drainage and economical issues. Famous pioneers include Frenchmen Hubert Gautier and Pierre-Marie-Jérôme Trésaguet as well as the Scottish engineers Thomas Telford and John Loudon McAdam, from whom the name "macadam" is derived[142, ch.5] [90, ch. 9].

However, these early modern roads were all unbound and dust became a severe problem with the advent of motor vehicles at the end of the 19th century. The low air pressure under fast-moving vehicles sucked dust from the road surface, created dust clouds, and lead to destabilisation of the road. By that time, remedies were at hand, though. Sir Walter Raleigh had been the first European to visit the La Brea Pitch Lake in Trinidad in 1595. In Europe, the physician Eirini d'Eirinis had discovered the natural asphalt deposits in La Presta in the Val de Travers in Switzerland in 1711. Other European sources of natural asphalt can be found in Seyssel and Lobsann in France, among others.

Early experiments with natural asphalt did not work out well for roads. First, Mastic Asphalt (Gussasphalt) (MA) was used, a mixture of melted powdered natural asphalt and tar, partly enriched with gravel or sand. These surfaces softened during summertime and have not been resilient enough due to insufficiently constructed base courses. Hence, asphalt usage was mostly restricted to sidewalks, which existed in this form in many European cities around 1840.

Therefore, it was soon decided to use stamped asphalt (crushed, but not powdered natural asphalt), developed by Swiss and French engineers de Coulaine, Mérian, Malo, and Vaudrey. Stamped asphalt had a lower bitumen content than MA, which made it less deformable at elevated temperatures. Also, the critical role of load-bearing base courses became known. Hence, this mixture was already applied on a concrete base course and then compacted by pounding to a thickness of only a few centimetres in Paris in 1854 . However, stamped asphalt roads were further compacted and polished over time, which proved to be disadvantageous. Vehicles and horses could easily slip, particularly on wet surfaces[194].

Tar competed with bitumen as a binder. In 1834, British John Henry Cassell, patented "lava stone", which consisted of a layer of tar, covered by a layer of macadam and sealed with a mixture of tar and sand [147]. In 1902, a Swiss physician, Ernest

²Cobblestone = rounded, unbroken stone. Sett = almost cuboidal quarried and machined rock.

Guglielminetti, approached the dust problem by spraying tar on the surface to create so-called tar-bound macadam [194]. The same year, Welsh civil engineer Edgar Purnell Hooley patented “tarmac” a mixture of coal tar and ironworks slag [37].

Modern rolled asphalt dates back to the Belgian chemist Edward de Smedt, who had emigrated to the United States. He employed Trinidad asphalt, which had a stiffer bitumen than the European deposits. Thus, he fluxed the bitumen with oils. Furthermore, the volcanic rock in Trinidad asphalt lead to surfaces with higher roughness than it was known from its European counterparts, as proven on a test-track in Washington in 1876. De Smedt was also probably the first to acknowledge the importance of a load-bearing granular scaffold and engineered a “well-graded” asphalt of maximum density. Also, layered road construction started in the US, as a patent filed in 1869 indicates. Advances in engineering lead to the development of mechanised mixing, installation, and compaction machinery, which drastically increased paving speeds.

Bitumen was increasingly distilled from crude oil. In order to assess product quality, standardised test methods became a necessity. The American Clifford Richardson developed — together with other researchers — the needle penetration test. It is still in use today, cf. section 1.2.3. He also advanced mix design with the demand for specifying the granulometric distribution with specialised sieves. The ring-and-ball test has been introduced in 1936, Fraaß breaking point one year later. The Marshall-test came into service in 1939. Due to growing importance of the granular scaffolding, special tests for the mineral aggregate have been developed. Fuller and Thompson were among the first to systematically investigate the Particle Size Distributions (PSD), or gradation, with the aims of dense mix and small granular surface. The basic equation is

$$P = \left(\frac{S}{S_{max}} \right)^n, \quad (1.1)$$

where P is the cumulative mass-percentage of rocks up to sieve size S , S_{max} is the maximum aggregate size, and n is a parameter that governs gradation. Fuller and Thompson [69] proposed $n = 0.5$ for maximum density. The US Federal Highway Association established the use of $n = 0.45$ in the 1960s, which is still in use today [148].

After WW2, the number of motorised vehicles drastically increased. In the US, it doubled between 1945 and 1955 [62]. This brought forth several problems with asphalt longevity, which led to the largest field trials of pavement construction methods to date, the AASHO³ road test [84]. This quickly separated good from bad designs and inter alia lead to the insight that the damage inflicted by a vehicle on roads grows with the fourth power of its weight.

Until the 1960s, asphalt concrete was the dominant mix type, which suffered severely from the increasingly popular spike tyres. Eventually, spikes were strictly regulated,

³Until 1973, the American Association of State Highway and Transportation Officials (AASHTO) was called the American Association of State Highway Officials (AASHO)[61].

but also new mix designs emerged which were less susceptible to wear and tear. The “well-graded” mix design gave way to “gap-graded” ones, with a high content of coarse grains, which could resist spikes. Stone Mastic Asphalt (SMA) was born, a mixture with particular requirements for hard-wearing and angular mineral aggregate. The coarse grains interlock to form a granular scaffold (stone skeleton) which inhibits permanent deformation. The gap-graded design features a high amount of voids in mineral aggregate (VMA), see section 1.3. This requires an increased bitumen content, which is stabilised with filler and fibres to form a so-called mastic in order to prevent run-off [90, ch. 12.3]. Nowadays, the aggregate in SMA consists of typically 75 m.% grains ≥ 2 mm [65].

Porous asphalt (PA) features an even more radical — almost monodisperse — particle size distribution with more than 90 m.% of coarse aggregate [65]. Here, the idea is to achieve a void network, which allows to drain water and disperse noise. First installations took place on airports. The reduced contact areas between neighbouring stones ask for strong binders with excellent adhesion properties. Thus, the advent of Polymer Modified Bitumen (PMB) boosted the use of PA, at least in regions with mild winters, since ice and PA is a problematic combination.

Nowadays, the vast majority of road pavements is constructed with asphalt.

1.2 Bitumen

Bitumen is a low-volatile, dark-coloured viscous liquid consisting of hydrocarbons and hydrocarbon derivatives, sulfur, oxygen, and nitrogen [35; 13]. In a simplified manner, bitumen can be characterised as a colloidal 2-phase material consisting of

- an oily phase: maltenes with a molecular mass of 500 g mol^{-1} to 1000 g mol^{-1} ,
- a dispersed solid phase: asphaltenes with a molecular mass of 5000 g mol^{-1} to $100\,000 \text{ g mol}^{-1}$.

The excellent waterproofing of bitumen is a result of its hydrophobic properties. It is furthermore chemically stable to most inorganic acids (exceptions: nitric acid HNO_3 and sulfuric acid H_2SO_4), bases and salts and strongly polar solvents such as alcohol and water. It is flammable at elevated temperatures, with a flashpoint of $\gtrsim 220^\circ\text{C}$. Bitumen is partially soluble or swelling in liquid hydrocarbons, such as gasoline, diesel, oils or other non-polar solvents e.g. toluene or trichloroethane [143].

1.2.1 Production

Pure bitumen does not occur naturally, but is industrially made by vacuum distillation of selected crude oils. In the process depicted in figure 1.2, crude oil is heated to temperatures between 300°C to 350°C to separate lighter fractions from the non-boiling

component. The latter is called atmospheric residue. The lighter fractions are used elsewhere. In order to remove the last traces of the lighter fractions, the atmospheric residue is then transferred to a vacuum distillation unit. The pressure reduction lowers the boiling point and avoids unwanted thermal cracking of the molecules. The pressure and temperature conditions within the vacuum process determine the hardness of the residue and thus the quality of the bitumen produced.

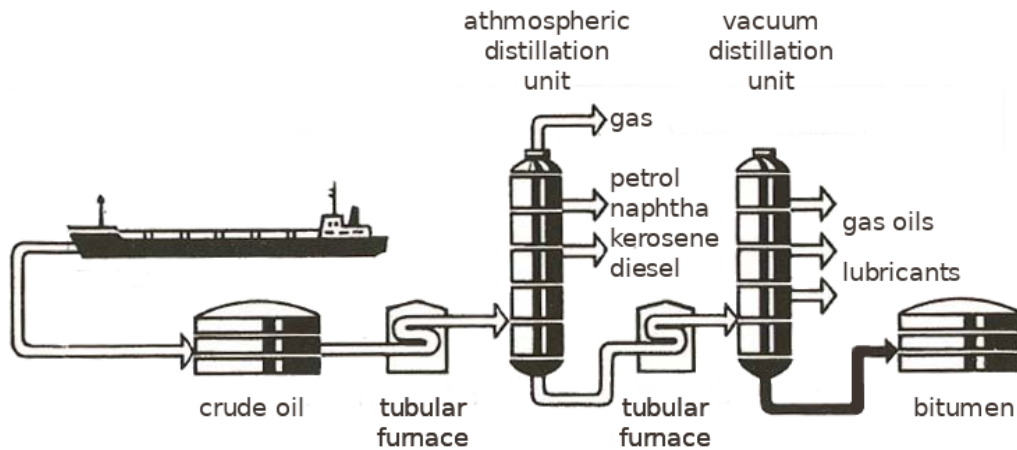


Figure 1.2: Schematic of the bitumen production process. Altered from source: Oeser et al. [139, p. 125]

1.2.2 Mechanical Properties

Bitumen is an elastoviscoplastic material with strong thermal dependence. It solidifies and becomes eventually brittle upon cooling; this is the so-called glassy state. During heating, it continuously goes through the stages of solid, then highly viscous, until it becomes a thin fluid at temperatures around 150 °C to 200 °C. At even higher temperatures, it starts to degrade. Unlike water, bitumen has no fixed melting point but exhibits a melting range, because the components of the hydrocarbon mixture have different melting points. The properties of bitumen change over time, it ages. The loss of volatile components at elevated temperatures and oxidation are regarded as the two main factors for these changes, which lead to increased stiffness and brittleness[86]. The increased stiffness can be beneficial at high surface temperatures, however, increased brittleness causes problems at low temperatures since stresses are no longer relaxed but cracking occurs [139]. Hence, damage is also a phenomenon that needs to be taken into regard. In principle, at temperatures above the glass transition regime,

bitumen can undergo tremendous deformations, which is strikingly demonstrated by the force ductility method, see section 1.2.3. However, during normal service, deformations are small and kinematic nonlinearity can be neglected. This also holds for asphalt. Although significant strain localisation takes place within the binder, or rather, the mortar (cf. section 3.6.2), deformations are still small. The sometimes huge deformations of ruts are the result of an incremental process that involved possibly thousands of tyre transitions and do not occur ad-hoc. In the following, the most frequently used characterisation methods are described.

1.2.3 Mechanical Characterisation

Due to the complex material properties, there exist several different (standardised) experimental setups to characterise bitumen. Some of them have been around for a long time. The advent of modern test equipment like Dynamic Shear Rheometry (DSR) will probably make some of the older tests obsolete in the future. Nevertheless, needle penetration and softening point ring and ball remain the two fundamental defining characteristics of bitumen produced to engineering specifications, as of today.

- Needle Penetration according to DIN EN 1426 [17]. Indicates hardness at 25 °C. It is used for classification. E.g. a 50/70 bitumen means that the needle sinks 50 dmm to 70 dmm into the bitumen specimen within 5 s. This is called the PEN grade. The terminology is extended for modified bitumen, see below.
- Ring and ball according to DIN EN 1427 [18]. Indicates softening point.
- Fraaß breaking point according to DIN EN 12593 [14]. Indicates brittleness at low temperatures.
- Ductility method according to DIN EN 52013 [1].
- Dynamic shear rheometer according to DIN EN 14770 [7]. Yields viscoelastic modulus, i.e. complex shear modulus and loss angle, see section 3.3, over temperature and/or loading frequency. Usually in linear viscoelastic regime.
- Rolling thin film oven test according to DIN EN 12607-1 [15]. Indicates short-term ageing during mix production.
- Pressure Ageing Vessel test according to DIN EN 14769 [5]. Indicates long-term ageing during service.

PMB [11; 13] is bitumen mixed with 3 m.% to 5 m.% polymers [90]. PMB has the advantage of easier workability (better compaction) during construction, it is stiffer at high temperatures (less rutting) and more viscous at low temperatures (less cracking). Furthermore, its adhesive and ageing behaviour is improved. [143; 139]. A typical

PMB label is 25/55-55A, where "25/55" indicates PEN grade, "55" indicates the softening point ring and ball and "A" means elastomer modification, usually in form of SBS (Styrene-Butadien-Styrene). Also plastomer modified bitumen exists (index "C"), although it is rarely applied [90]. EVA (Ethene-Vinyl-Acetate) and PE (Polyethylene) are examples of commonly used plastomers. Two additional tests exist for PMBs.

- Elastic recovery according to DIN EN 13398 [23].
- Tensile properties using the force ductility method according to DIN EN 13589 [24].

1.3 Mineral Aggregate

Asphalt mixtures contain 92 m.% to 96 m.% mineral aggregate [90, ch. 2.7]. Thus it is worthwhile to source local aggregate since its volume and weight render transportation costly. There are no particular requirements concerning the type of rock. However, the aggregate has to be strong, hard-wearing, insensitive to moisture, and it has to have a high affinity to bitumen. Regarding morphology, grains need to have a high amount of crushed faces and aspect ratios should not be too high. Morphology is thoroughly analysed in section 4. In Germany, the technical terms of delivery for aggregates used in road construction [64] regulate how European standards ([16]) are put into practice and references more specific standards. Concerning the nomenclature, the following definitions hold:

- Coarse aggregate (rock): retained on 2 mm sieve.
- Fine aggregate (sand): passing the 2 mm sieve, but retained on the 0.063 mm sieve.
- mineral filler: passing the 0.063 mm sieve.

1.3.1 Particle Size Distribution

As already mentioned, the PSD is particularly important for the formation of a load-bearing granular skeleton. As there are asphalts following different concepts, each has its own specific PSD. The technical terms of delivery for asphalt mixes for the construction of asphalt pavements [65] provide the PSDs, cf. figure 3.12. A flexible algorithm for the generation of different PSDs is proposed in section 3.

1.4 Asphalt

Asphalt is a composite material consisting of bitumen, mineral aggregate⁴, voids, and sometimes additional fillers, such as cellulose fibre. It inherits most of its mechanical properties from bitumen, but with the notable difference, that it behaves more solid-like at elevated temperatures, than pure bitumen does. According to Oeser et al. [139], the main requirements are:

- **Stability:** No permanent deformations under load.
- **Crack resistance:** Sufficient viscosity at low temperatures to relax stresses. Characterises mostly top-down cracking.
- **Fatigue resistance:** Enduring load in high cycles without cracking. Characterises mostly bottom-up cracking.
- **Installability:** Transportation and installation without demixing. Good compactibility.

The surface course is directly exposed to traffic and environment. Hence, it has particular requirements regarding:

- **Impermeability:** Water must not enter the surface course. Notable exception: porous asphalt.
- **Durability:** Resistance to wear and tear; weather conditions.
- **Road safety:** Constantly good grip, low noise level.

1.4.1 Characterisation

There is a plethora of test methods, particularly for HMA (DIN EN 12697-1–43), and it is not possible to present all of them here. The most important ones necessary for dimensioning according to German pavement design guideline (RDO Asphalt 09) are

- Stiffness according to EN 12697-26 [21].
- Fatigue resistance according to EN 12697-24 [20].

⁴mineral filler, fine and coarse aggregate

1.5 Mix Design

The quality of the ingredients is critical for the quality of the resulting mix. However, it is worthwhile to use cheap ingredients and thin layers for economic reasons. Thus, it is necessary to tailor mix design to the unique performance requirements dictated by the traffic, climatic, and structural conditions at a particular construction site [48].

For most types of asphalt, the air void content is an important design variable. It must be high enough to yield durable bitumen film thicknesses around the grains, and it must be low enough not to compromise load transfer via the granular skeleton. figure 1.3 shows a depiction from the US Superpave Mix Design Manual [48].

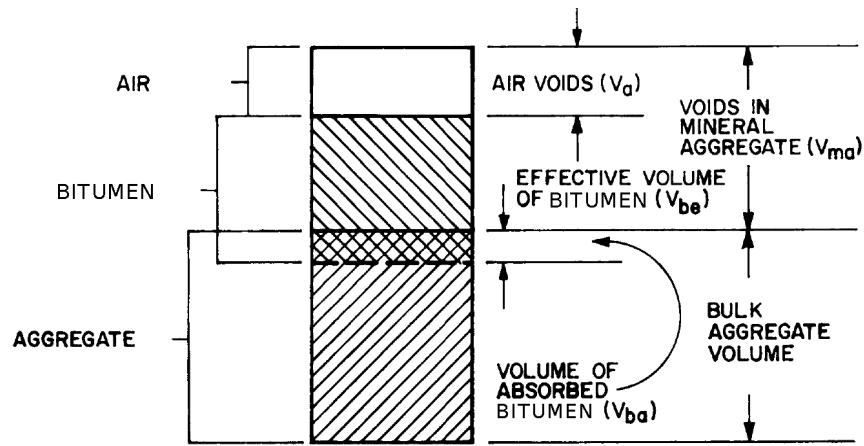


Figure 1.3: Asphalt mix design according to Cominsky et al. [48, Fig. 3.2]. Labels altered from source.

The bulk aggregate volume includes both the volume of the impermeable portion of the aggregate particles and the volume of the permeable voids in the particles, but not the volume between particles. The bulk volume of the aggregate is equal to the volume of water displaced by the aggregate in a saturated, surface-dry condition. A fraction of the bitumen infiltrates the permeable voids, this is the volume of absorbed bitumen, V_{ba} . The difference of the total bitumen volume and V_{ba} is the effective volume of asphalt V_{be} , which can glue grains together. Together with the air voids, V_a , V_{be} is the volume of voids in mineral aggregate, V_{ma} . Although no mixes have been tested for the present work, DSR has been used to characterise the linear viscoelastic behaviour of bituminous mortar. Mortar design follows similar considerations as mix design, see section 3.3.1. In hindsight, there is a conceptual mistake in the mortar design as will be discussed in section 5.2.

1.6 Pavement Construction

Modern Roads have a layered construction so that each layer is tailored to its own specific purposes, while keeping costs at bay. The lifetime of a road increases exponentially with total thickness[90, ch. 10]. Hence, it is the purpose of the dimensioning process to balance longevity and costs, based on traffic and weather conditions[10; 3].

Most roads are constructed on levelled and compacted soil (compacted subgrade), over which an unbound subbase course is raised. This subbase course mainly serves drainage to prevent frost and thaw damage. Then, the bound base course is paved; it connects the surface course to the subbase. Its main objective is to distribute the loads from the surface evenly into the subbase, so as not to exceed admissible foundation pressures (EV2). Soil which is less capable of bearing a load requires thicker base courses. The passing traffic causes cyclic flexural tension at the bottom of the base course. A typical failure pattern is that cracks develop from flexural tension and move upward until they appear at the road surface. Hence, strength of the this layer is critical. Depending on the destined load level, there can be a so-called binder course above the base course. Its purposes are the improvement of evenness and load-bearing, as well as to distribute the high traffic-induced shear-stresses. The surface course is directly exposed to the traffic, weather conditions, and de-icing agents. Therefore, it has special requirements like grip, evenness, and wear-resistance. This layer has the most demanding requirements to the mineral aggregate, such as roughness, to prevent skidding, angularity and resistance to fragmentation for grain interlocking and stability [90, ch. 12].

2 Computational homogenisation from a 3D finite element model of asphalt — linear elastic computations

This article was published as:

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J. Wimmer devised and implemented the geometry model generation in **Matlab**, ran the simulations, interpreted the data, and wrote the article.

B. Stier implemented the periodic boundary generation in **Abaqus**.

J.-W. Simon and S. Reese provided intellectual content and gave conceptual advice.

S. Reese was engaged in obtaining funds for the research.

All authors drafted the work for intellectual content.

All authors approved the publication of the final manuscript.

Note: The terminology has been unified. Asphalt concrete is now called asphalt.

2.1 Abstract

Asphalt is a composite material consisting of bituminous binders, mineral aggregate, and voids. Experimental and computational efforts to assess the bulk mechanical properties of asphalt ubiquitously raise the question of representative sample size. It is well known that the dimension of a sample has to be larger than the largest morphological entity. However, it has been shown that the required size is a function of the morphological and physical properties under consideration, e.g. the difference between the properties of the constituents at the microscale, and their volume fractions. In the present contribution, representative sample sizes are determined numerically for a variation of parameters in terms of a tolerable amount of statistical scatter by conducting virtual experiments. If the scatter between distinct heterogeneous samples falls below a certain threshold, the corresponding volume is called a Representative Volume Element (RVE). Finite element (FE) discretisations of asphalt volume samples are generated by means of a shrunk Poisson Voronoi tessellation. In order to provide estimates for the evolution of the RVE size under changing material properties of the mortar, the stiffness ratio between rocks and mortar is varied by two orders of magnitude. Furthermore, the influence of a variation in volume fraction is investigated.

2.2 Introduction

Whether or not a material should be treated as a composite can be considered as a question of the scale of interest. A small enough scale will reveal heterogeneities in almost any material. In order to get a better understanding of the bulk characteristics of a material, it is important to study and understand its microstructure. Thus, there is a need to create a mesomechanical virtual laboratory for asphalt to estimate its effective properties. The bulk behaviour of asphalt does not only depend on the material properties of its constituents, but also on structural properties such as shape, granulometric and orientation distributions [60]. In order to assess the impact of changes of the structural composition, the reconstruction of the structure from image data is not suitable. Rather, a flexible methodology to randomly generate structures that resemble asphalt is needed for this purpose. The effective properties can be thought of as the properties observed for testing a specimen of infinite dimensions, which contains all microheterogeneities characteristic to the material in an infinite number. Otherwise, material properties will always be mixed up with structural properties. For the testing — be it real or virtual — of specimens of finite dimensions, a compromise between effort and accuracy has to be found. Therefore, it is desirable to establish lower bounds for the specimen size that still allow to call it a representative volume element. As Huet [89] and Kanit et al. [96] point out, the RVE size is a function of

the morphological or physical property under consideration. In the present study, it is a function of the contrast in the properties of the microconstituents, and their volume fractions.

Current approaches to computational modelling of asphalt can be separated in continuum, mesoscale, and multiscale approaches. The terminology used throughout the present study is the following: Continuum approaches do not explicitly model the granular structure of asphalt, but treat the composite in a smeared fashion [55; 138; 128]. Mesoscale models take the grains explicitly into account via a geometric representation [125; 184; 192; 175]. Multiscale models are bridging the gap between mesoscale and continuum approaches by performing homogenisation from the smaller scale to obtain smeared parameters for the use at the continuum scale [117; 60; 102; 156]. This classification neglects that mesoscale models usually employ a size threshold of geometric modelling and treat only a fraction of the grain size distribution explicitly. In the context of asphalt, this means that small grains are mixed with the bitumen. The properties of this mixture are represented in a smeared way by considering a continuous mortar phase.

The importance of conducting full 3D analyses of asphalt behaviour is highlighted, for example, by Mo et al. [127], who find that their 2D model underestimates the stresses in the mortar by a factor of 2.6 – 3.5. This is supported by the research of Fakhari Tehrani et al. [59], who conclude that experimental results of the complex modulus of asphalt mixtures are better reproduced by 3D approaches. Since computational resources are easily overpowered by 3D mesoscale simulations, for example, of moving wheel loads [127], the need for efficient computational homogenisation arises. The present work provides a first step towards a virtual laboratory that enables both mesoscale investigations and upscaling of homogenised properties to computationally efficient continuum approaches.

Periodicity is a feature of paramount importance for computational homogenisation from RVEs. It has been shown by various researchers, that displacement (Dirichlet) boundary conditions (BCs) overestimate the effective material properties, whereas traction (Neumann) BCs underestimate them. Although the advantages of one type of BC over the other diminish with increasing RVE size it is worthwhile to keep the computational effort to a minimum. The superior performance of displacement based PBCs for the prediction of effective properties has been demonstrated analytically [88; 89; 140] and numerically [124], [96; 156], see Nguyen et al. [135] for a review. However, the application of PBCs requires the geometry, as well as the Finite Element (FE) mesh, to be periodic at the boundaries.

FE based investigations to determine minimal RVE sizes for randomly generated structures have been performed for several materials. As the research field of computational homogenisation has experienced tremendous growth in recent years, only a few selected publications will be discussed here. The interested reader is referred to Nguyen et al. [135] for a broader discussion of the topic. Synthetic geometries are

frequently used for the multi-scale simulation of metals. Fritzen et al. [68] investigate the convergence of effective properties for gold, nickel and copper by means of Voronoi tessellations. They later extend their methodology to metal-matrix composites [67]. They apply a method to shrink Voronoi cells in order to create space for a matrix, in which the particles are suspended. Periodicity of geometry and mesh is established and the required size is determined for a material contrast of ≈ 5.7 and particle volume fractions of $0.1 - 0.8$. The applicability to high contrast materials is assessed for a stiffness ratio of 100, without investigating RVE convergence. Kanit et al. [96] thoroughly investigate convergence of a 3D dual-phase structure based on a neat Voronoi tessellation with contrasts of 100 and 1000 and volume fractions between $0.525 - 0.725$. Shahzamanian et al. [158] determine the RVE size for a multi-phase cement paste based on block meshes. Stroeven et al. [162] employ the discrete element method to create structures of spherical matrix inclusions. The material contrast is ≈ 2.86 , and the volume fraction ranges from $0.3 - 0.75$. Wriggers and Moftah [181] create random sphere based models for the simulation of concrete. Their approach considers the granulometric curve. 3D computations are used to determine the effective properties. Savvas et al. [153] study the homogenisation of structures with arbitrarily shaped inclusions by means of the extended finite element method. They investigate values of material contrast up to 1000, and volume fractions between $0.2 - 0.4$.

Several researchers do not generate synthetic geometries, but digitalise real geometries from image data. Only few investigations of representativeness are conducted. RVE sizes for human cortical bone have been determined by Grimal et al. [78] based on acoustic microscopy. Kanit et al. [97] investigate two different materials from food industry, based on 3D confocal images. Digitalisation from image data is common in the context of asphalt. 2D models can be generated from simple images [120; 44; 174; 32]. Tashman et al. [165] enrich continuum modelling of asphalt with a microstructure tensor that allows to take mesostructural geometric properties into account without explicit discretisation. Kim et al. [101] conduct an experimental and FE-based study on determining RVE sizes for the viscoelastic dynamic modulus of three different asphalt mixtures. Sinusoidal Dirichlet BCs are applied. They conclude that RVE dimensions have to be approximately four times larger than the nominal maximum grain size. Mitra et al. [125] perform 2D nonlinear viscoplastic simulations of the indirect tensile test. In their work, the results obtained from a random ellipsoid inclusions model are compared to results from an image based structure. They conclude that image based modelling does not offer significant advantages over their synthetic sample. 3D reconstructions of real asphalt geometries typically rely on computer tomography [177; 105; 184].

Synthetic approaches to create asphalt mesostructures are frequently based on spheres/ellipsoids [127; 92; 51; 156] and polyhedra [100; 116; 192; 102; 175]. A noteworthy contribution has been made by Fakhari Tehrani et al. [60], who employ a structural model generator for 2D mesoscale modelling of asphalt. Their approach captures the granulometric

curve and allows the investigation of the influence of irregular polygonal over spherical particles. A mesh density study is performed and the numerically determined complex modulus is compared to experimental results.

The present paper demonstrates a methodology to generate 3D synthetic structures of asphalt based on Voronoi tessellations and the computation of effective properties by means of homogenisation techniques. Periodicity is enforced in the geometry, the mesh, and through the application of PBCs. The sample size required for representativeness is determined numerically through a statistical measure of convergence. The two phases, rock and mortar, are modelled as linear elastic. Based on a threshold of the granulometric curve, volume fractions of rock and mortar for a German standard SMA are established. Inelastic material modelling of the bituminous mortar phase is out of scope of the present paper. Nevertheless, linear elastic modelling allows to show the validity of the methodology and furthermore highlights the influences of volume fraction and the contrast of material properties on RVE size.

The outline of the article is as follows: section 2.3 discusses the generation of periodic geometry and mesh for the example of asphalt. In section 2.4, the realisation of specific volume fractions and the material properties are presented. A statistical measure of convergence is introduced in section 2.5, followed by the results for all examples in section 2.6.

2.3 Microstructural Modelling of Asphalt

The geometry generation for mesostructural models of asphalt is independent of its mechanical quantities. On the other hand, estimations of the overall mechanical behaviour are only possible in combination with constitutive laws for the rocks, the bituminous mortar gluing the composite together, and their interaction. Thereby, aspects such as rate-dependence and thermomechanical coupling would be important for the modelling of bituminous binders/mortars. This is, however, out of the scope of this paper.

Modern road engineering has developed a plethora of different asphalt types in terms of rock/binder ratio, grain size distribution and binder type. For example, asphalt on bridges must not be vibration rolled, hence it is “softer” than most other mixtures, and some asphalt types are open porous to increase drainage and reduce noise. Hence, computational modelling of asphalt geometries should be flexible enough to capture a variety of mixtures. Current mesostructural approaches cannot take the whole particle size distribution of asphalt into account for reasons of computational feasibility. Typically, the small aggregate fractions are assigned to a bituminous mortar phase, subsequently modelled as a continuum. Definitions of the size threshold for the mortar phase vary. Typical choices are 0.5 mm [180], 2 mm [26], 2.36 mm [51; 174; 125; 192; 59], and 4.75 mm [175]. Here, the 2 mm threshold is adopted and applied to the

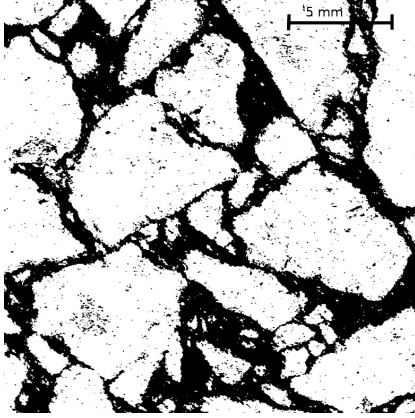


Figure 2.1: Close-up of German standard SMA 11 S asphalt.

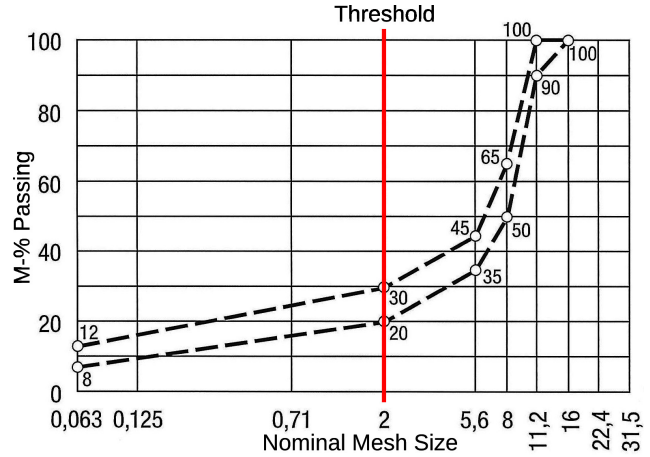


Figure 2.2: German standard SMA 11 S granulometric curve. The threshold divides the continuum phase on the left, from the discretely modelled one on the right. Taken from [65] and modified.

example of German standard stone mastic asphalt with 11 mm maximum aggregate size: SMA 11 S. A closeup of a cut through SMA 11 S is depicted in figure 2.1, and its granulometric curve is given in figure 2.2. The adjustment of the Voronoi tessellation to fit prescribed particle size distributions will be described in another publication.

2.3.1 Voronoi Tessellations

Existing approaches to model granular materials with irregularly shaped particles are based on different types of Voronoi tessellations, see e.g. Aurenhammer [34] for an overview. The input to a Voronoi tessellation is an arbitrary distribution of n seeds in a domain D . A projection of seeds and a yellow coloured cubic domain into the x-y plane is depicted in figure 2.3. If a random distribution is chosen, the term Poisson Voronoi tessellation is used. It is this randomness that causes scatter in the homogenised properties. A periodic tessellation is enforced by generating the seeds randomly within D and copying them around the domain 26 times, as proposed by Decker and Jeulin [54]. The Voronoi tessellation is generated using `Matlab` [122]. Extensive use is made of the `geom3D` package [113] for creating minimal convex hulls based on `qhull` [36] and numerous geometric operations. The peculiarity of the Voronoi tessellation is that

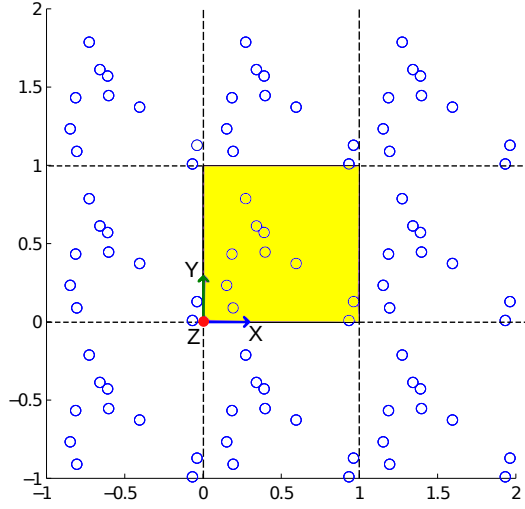


Figure 2.3: View in z-axis direction of the randomly distributed seeds and the domain. The periodicity of the seeds enforces a periodic Voronoi tessellation.

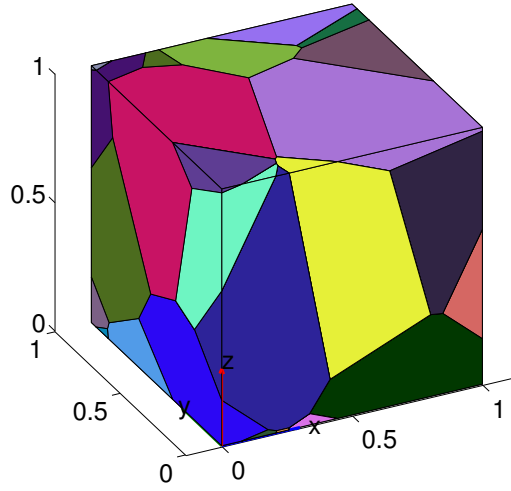


Figure 2.4: Neat Poisson Voronoi tessellation trimmed to cubic domain.

every point P within a certain region V_i is closer to its seed S_i , than to any other seed S_j :

$$V_i = \{P \in D | d(P, S_i) < d(P, S_j), \forall i \neq j\}^1. \quad (2.1)$$

Here, d is the distance as given by a certain metric. Depending on the choice of metric, the Voronoi tessellation looks differently. By using the Euclidean distance, the domain is divided into convex polyhedra, see figure 2.4. A critical view at typical asphalts (see figure 2.1) proves that convexity does not hold strictly. Nevertheless is the assumption of convexity common in the modelling of asphalt and regarded as a minor idealisation. The Voronoi tessellation has physical justification for the modelling of some metals. In the context of asphalt, it is merely chosen for reasons of visual resemblance.

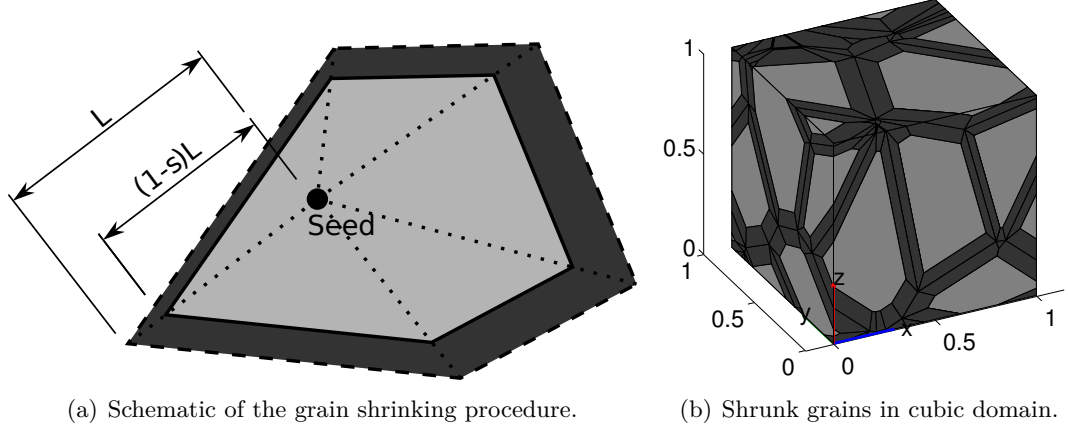


Figure 2.5: Illustration of the shrinking procedure. figure 2.5(b) shows the same structure as figure 2.4, but with shrunken cells. The mortar layer thickness between face pairs is constant, but not within D .

2.3.2 Shrinking of Polyhedra

In a neat Voronoi tessellation as depicted in figure 2.4, the grains² touch seamlessly. In order to create space for the bituminous mortar, the original Voronoi polyhedra are undergoing a shrinking procedure. Subsequently, the free space is filled by new polyhedra representing the mortar. The procedure is illustrated in figure 2.5(a), and the result of shrinking the grains of the structure shown in figure 2.4 is depicted in figure 2.5(b). For a given grain, all vectors from its seed to the nodes are computed and scaled by a shrinking factor $0 < s < 1$. Using this procedure, the facets of neighbouring grains remain parallel to each other and the thickness of the mortar layer is not constant throughout the domain, but per face pair. Please note that the shrinking procedure could be carried out using any point lying within the grain, therefore changing the geometric properties of the layer. Also, the shrinking factor could vary from grain to grain, but not within one grain, as this would violate convexity of the polyhedron. Nevertheless, a constant s is chosen throughout this study for reasons of simplicity. This method varies from the erosion process used by Fritzen and Böhlke [67] in several regards. In the present approach, the thickness of the layer

¹This is the definition used e.g. by Du et al. [56]. Mathematically, this definition creates a set of points which does not belong to any polyhedron, but constitutes its boundary which is used to define the polyhedron.

²From a mathematical point of view, the Voronoi cells are convex polyhedra. However, from a road engineering perspective, the Voronoi polyhedra are representing the grains within asphalt. Henceforth, both terms are used interchangeably.

between neighbouring grains is not constant throughout D . It appears from visual inspection, that constant mortar thickness is untypical for asphalt (cf. figure 2.1). Furthermore, the present approach does not employ an iterative procedure to obtain a certain volume fraction. After the grains have been shrunk, the Voronoi tessellation is trimmed to desired domain shape and the convex hulls of all trimmed polyhedra are updated. Given a constant shrinking factor, simple geometric considerations allow to write the total rock volume V_R by means of the equation

$$V_R = V_T(1 - s)^3, \quad (2.2)$$

where V_T is the total volume of the domain. In a periodic Voronoi geometry, the number of grains matches exactly the number of seeds lying within the domain. The nominal number of grains is higher, but if one takes into regard that grains intersecting the domain boundary continue on the opposite face of the RVE, the effective grain number, n , is obtained. In order to obtain the “correct” material response, the required RVE size has to be determined. We follow the convention used by Kanit et al. [96] to fix the mean grain volume V_{G_m} to unity: $V_{G_m} = 1$. That is $V_R = n \times V_{G_m} = n \times 1$. Hence an increase in V_T is analogous to an increase of n . Please note that the absolute domain size does not matter for the identification of RVEs. It is also possible to keep V_T fixed at an arbitrary value and treat V_{G_m} as a function of n . However, the accuracy of geometric operations should be kept in mind when choosing the absolute domain size. By using (2.2), V_T can be expressed as

$$V_T = \frac{n}{(1 - s)^3}. \quad (2.3)$$

2.3.3 Meshing

Periodic quadratic tetrahedral meshes are created by the open-source mesh generator GMSH [76], see figure 2.6 for a depiction of a meshed volume element. It pursues a hierarchical meshing procedure by first creating a 1D mesh on the edges of the structure. This imposes a constraint on the 2D mesh of all facets and likewise on the full 3D mesh for volumes. Given a deterministic behaviour of the meshing algorithm, meshes of identical facets will be identical. It is well known that neat Voronoi tessellations are badly conditioned for meshing. This is due to the fact that a Voronoi tessellation produces some edges and facets that are extremely small compared to the characteristic length of the structure. Furthermore, trimming introduces additional disadvantageous geometric properties like thin layers and small dihedral angles. The presently generated meshes can clearly be improved. Particularly large elastic and/or inelastic strains are prone to require higher mesh quality.

Mesh convergence has been checked for a high material contrast using a rock volume fraction of $\Phi_R = 0.73$ and 9 seeds. Only the mesh density is changed, the geometry

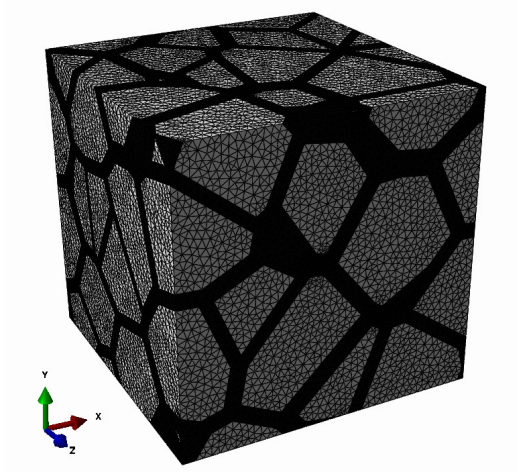


Figure 2.6: Tetrahedral mesh of a volume element with 30 grains and $\Phi_R=0.63$.

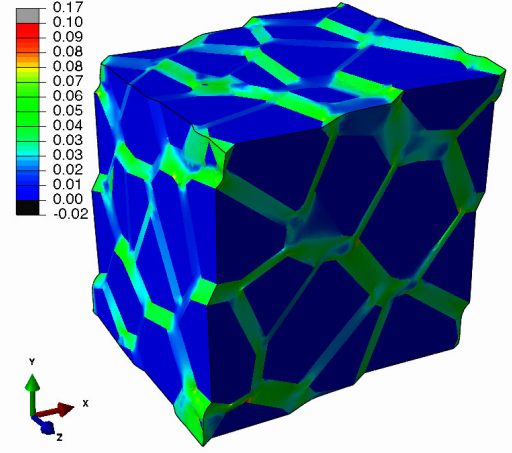


Figure 2.7: 20 times exaggerated ϵ_{xy} of the VE shown in figure 2.6. A far-field strain of $\epsilon_{xy} = 0.01$ was applied.

for all computations remains the same. figure 2.8 shows the results. The finest mesh has 2155980 degrees of freedom corresponding to a characteristic length of a single tetrahedron of 0.05. The discretisation error

$$err = \frac{\bar{E}_c - \bar{E}_f}{\bar{E}_f}, \quad (2.4)$$

where the subscripts f and c denote the finest and a coarser mesh, respectively, quantifies the relative change in mechanical response between different meshes. It is found that a characteristic element length of 0.1 is necessary to obtain $err \leq 2\%$. This is the characteristic element length used throughout the paper. Linear tetrahedra were found to require drastically finer discretisations and lead to higher computational effort.

It is noteworthy that the tetrahedron size is relatively homogeneous throughout the domain, except where small geometric details need to be captured by the mesh. However, a fine mesh is only necessary within the soft binder between harder particles, since strains localise here, and the mesh inside rocks could be coarse. This could either reduce the degrees of freedom substantially or allow for higher resolution within the binder. It is hypothesised that mesh convergence is governed by the binder mesh, particularly for high c_{RM} .

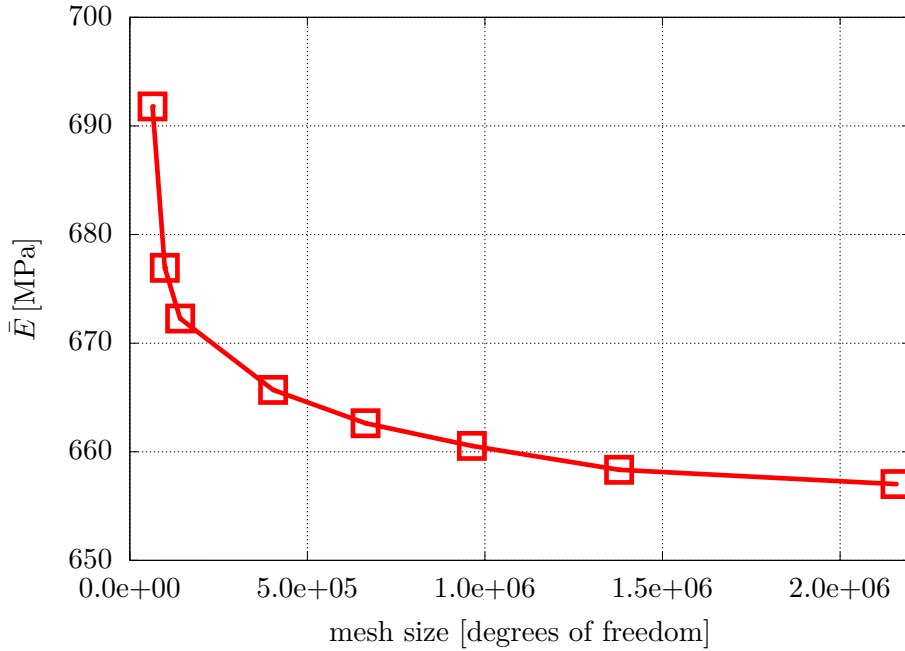


Figure 2.8: Behaviour of mean Young's modulus for an increasing number of degrees of freedom with $n = 9$, $\Phi_R = 0.73$, and $c_{RM} = 1000$.

2.4 Material Characterisation

The microconstituents exhibit a high variability in terms of material and morphological properties. For example, it is known that the material contrast of mortar to bitumen spans several orders of magnitude, depending on temperature, type of binder, volume fraction and mineralogy [126]. Likewise, the contrast between rocks and mortar, c_{RM} , is tremendous. A real bituminous mortar is a thick viscoplastic paste and its properties are — among other factors — strongly dependent on temperature and loading frequency. For example, Fakhari Tehrani et al. [59] provide contrasts of rock modulus, E_R , to the complex modulus of mortar of 22–9644, for loading frequencies of $10^{-2} - 10^{+5}$ Hz. Since experimental data of mortar behaviour with 2 mm size threshold are unavailable, the mortar is modelled as linear elastic. Its Young's modulus, E_M is implicitly defined as a fraction of the rock's modulus, see table 2.1. Its Poisson's ratio is simply chosen to be the arithmetic mean between the Poisson's ratios of rock and pure bitumen, which is typically assumed to be incompressible. In order to assess the non-constant mortar stiffness, RVE sizes are determined numerically for values of E_M which are one to three orders of magnitude lower than E_R . The pivotal quantity is the material/stiffness contrast, $c_{RM} = \frac{E_R}{E_M}$.

Dolerite, or diabase, is a typical rock type used in road engineering. It has a specific gravity of approximately $\rho_R = 2.8 \text{ g/cm}^3$. Together with the specific gravity of bitumen $\rho_B = 1.05 \text{ g/cm}^3$, and neglecting the presence of voids these data allow the computation of V_R for a given bitumen content. Here, the bitumen mass fraction is taken from [65] to be $\chi_B = 6.7\%$ [w/w]. SMA 11 S furthermore contains about 0.3% [w/w] fibres, but their influence on the total mixture density is negligible. Thus, the total mixture density is obtained as

$$\rho_{total} = \frac{\sum_i m_i}{\sum_i V_i} = \frac{1}{\left(\frac{\chi_b}{\rho_b} + \frac{(1-\chi_b)}{\rho_R}\right)} = 2.56 \text{ g/cm}^3. \quad (2.5)$$

By taking the mean of the total mass percentage of rocks withheld by a 2 mm sieve to be 75% [w/w] (see figure 2.2), we obtain the volume of rocks $> 2 \text{ mm}$ to be

$$V_{R>2mm} = \frac{m_{R>2mm}}{\rho_R} = 0.75 \times 0.93 \times V_{total} \times \frac{\rho_{total}}{\rho_R}. \quad (2.6)$$

The geometrically modelled rock volume fraction Φ_R is then obtained as

$$\Phi_R = \frac{V_{R>2mm}}{V_{total}} = 0.75 \times 0.93 \times \frac{\rho_{total}}{\rho_R} = 0.63. \quad (2.7)$$

By rewriting (2.2), s becomes a function of Φ_R

$$\begin{aligned} \Phi_R &= (1 - s)^3 \\ \Leftrightarrow \quad 1 - \sqrt[3]{\Phi_R} &= s = 0.1427. \end{aligned} \quad (2.8)$$

Furthermore the standards do not require strict bounds for the sieve residues, but allow rather loose bounds of 70–80 [%w/w] at 2 mm sieve spacing for SMA 11 S, see figure 2.2. In order to pay respect to these uncertainties, the current model is not overly exact in matching a certain parameter, but rather highlights a trend. First, in section 2.6.1, c_{RM} is varied by 2 orders of magnitude (see table 2.1) while keeping Φ_R constant. Second, in section 2.6.2, five different volume fractions Φ_R (see table 2.2) are investigated for a fixed c_{RM} .

2.5 Homogenisation Procedure

Periodic displacement based BCs have been implemented using a `Python` script for use with `Abaqus R2012a` [52]. For each of the investigated microstructures defined by a unique parameter set (n, Φ_R) , $N = 15$ samples are randomly generated to obtain homogenised values and perform statistics. Identical geometries are used for the investigation of the impact of c_{RM} . A far-field strain of 1% is applied to the samples in three uniaxial strain and three shear deformation modes in order to fully

Parameter	Value
E_R	80 000 MPa
ν_R	0.2
E_M	80 & 800 & 8000 MPa
c_{RM}	1000 & 100 & 10
ν_M	0.35

Table 2.1: Linear elastic material parameters for asphalt.

Φ_R	s
0.33	0.309
0.43	0.2452
0.53	0.1907
0.63	0.1427
0.73	0.09959

Table 2.2: Rock volume fractions and associated shrinking factors.

populate the elasticity tensor $\mathbb{C}$, cf. figure 2.7. For details about the application of PBCs, see Bednarczyk et al. [38]. In the following, the convergence behaviours of the mean Young's modulus $\bar{E}$ and the mean shear modulus $\bar{G}$ are investigated. They are computed by means of

$$\bar{E} = \frac{1}{N} \sum_{i=1}^N \frac{1}{3} (E_1 + E_2 + E_3)_i, \quad \bar{G} = \frac{1}{N} \sum_{i=1}^N \frac{1}{3} (G_1 + G_2 + G_3)_i, \quad (2.9)$$

where the index i refers to the current sample. The Young's and shear moduli are obtained from $\mathbb{C}$ (given in Voigt-notation) by

$$E_j = \frac{1}{(\mathbb{C}^{-1})_{jj}}, \quad j = 1 \dots 3, \quad G_{j-3} = \frac{1}{(\mathbb{C}^{-1})_{jj}}, \quad j = 4 \dots 6. \quad (2.10)$$

Since the response of an RVE must not depend on its orientation in space, the notions E_j and G_j become meaningless. In order to quantify the remaining anisotropy, the 2×3 effective moduli are sorted by size for each realisation, before computing the statistics for all 15 realisations of one set of parameters. For example, the mean of the largest Young's moduli between different realisations is given by

$$\bar{E}_+ = \frac{1}{N} \sum_{i=1}^N (\max E_j)_i, \quad j = 1 \dots 3. \quad (2.11)$$

It holds analogously for G . These major (+), middle (o) and minor (-) moduli should converge to the same value. Please note that these apparent moduli depend on the specimen orientation and thus are in general not the extremal moduli. Only in the limit case $n, N \rightarrow \infty$ true isotropy is obtained, and the apparent become the effective moduli. A different method to assess the deviation from isotropy in finite specimen sizes is presented in the following paragraph.

In order to obtain one quantity that captures both the scatter of the three (Young's) moduli obtained from the same specimen — i.e. the anisotropy — and the scatter be-

tween different realisations, the standard deviation takes $3 \times N$ arguments. Furthermore, the standard deviation, sd , is defined as the square root of an unbiased estimator of the variance of the population from which the samples are drawn:

$$sd(E) = \left(\frac{1}{3N-1} \sum_{i=1}^{3N} (E_i - \bar{E})^2 \right)^{\frac{1}{2}}. \quad (2.12)$$

It holds analogously for G . Through the use of Poisson-distributed seeds, the drawn samples are independent of each other.

2.5.1 Isotropy of Mean Apparent Moduli

The procedure proposed in the previous section is only one of the many methods to derive elastic constants from $\mathbb{C}$. Another one is to use isotropic projection on $\mathbb{C}$. The stiffness tensor can be additively decomposed into the projector representation [151; 150; 80]

$$\mathbb{C} = \sum_{\alpha=1}^{\beta} \lambda_{\alpha} \mathbb{P}_{\alpha}, \quad (2.13)$$

where $2 \leq \beta \leq 6$ is the number of distinct eigenvalues, λ_{α} , of $\mathbb{C}$. In the case of isotropic material behaviour, $\mathbb{C}$ possesses two distinct eigenvalues and the projectors are defined as

$$\mathbb{P}_1 = \frac{1}{3} \mathbf{I} \otimes \mathbf{I}, \quad \mathbb{P}_2 = \mathbb{I} - \mathbb{P}_1, \quad (2.14)$$

where $\mathbf{I}$ is the second-order identity and $\mathbb{I}$ is the fourth-order identity on symmetric second-order tensors. These projectors allow to obtain the bulk modulus $3K = \mathbb{C} : \mathbb{P}_1$ and the shear modulus $10G = \mathbb{C} : \mathbb{P}_2$. The Young's modulus is then given by $E = 9KG/(3K + G)$. Furthermore, the isotropic part of an effective stiffness tensor,

$$\mathbb{C}_{iso} = \lambda_1 \mathbb{P}_1 + \lambda_2 \mathbb{P}_2, \quad (2.15)$$

allows to obtain the anisotropic part as

$$\mathbb{C}_{aniso} = \mathbb{C} - \mathbb{C}_{iso}. \quad (2.16)$$

By computing the norms of $\mathbb{C}$ and its anisotropic part, $\mathbb{C}_{aniso}$, a degree of anisotropy, κ_{aniso} , can be defined as

$$\kappa_{aniso} = \frac{\|\mathbb{C}_{aniso}\|_F}{\|\mathbb{C}\|_F}. \quad (2.17)$$

Here, the subscript F indicates the Frobenius-norm. A small κ_{aniso} highlights that the direction dependence of the obtained elastic constants vanishes.

In the following, the influence of N is assessed. Several stiffness tensors for nine grains ($n = 9$), a material contrast of $c_{RM} = 1000$, and an increasing number of realizations ($N = 1, 5, 15, 30$) are given in Voigt-notation. The derived elastic constants, $\bar{E}_P$ and $\bar{G}_P$, obtained by using the projectors (2.14), κ_{aniso} and the elastic constants obtained by using (2.9) are shown. Where applicable, the standard deviation according to (2.12) of the respective elastic constant is displayed as well.

$$\mathbb{C}_{\substack{n=9 \\ N=1}} = \begin{bmatrix} 813.13 & 243.1 & 269.75 & -23.47 & -8.05 & 2.42 \\ & 792.06 & 294.93 & 4.98 & 13.23 & -23.71 \\ & & 809.69 & 19.56 & -15.37 & 9.03 \\ & & & 247.21 & 6.84 & 8.42 \\ & \text{Sym.} & & & 273.4248 & 19.22 \\ & & & & & 314.9 \end{bmatrix} \text{ MPa}$$

$$\begin{aligned} \bar{E}_P &= 683.26 \text{ MPa} \\ \bar{G}_P &= 274.25 \text{ MPa} \\ \kappa_{aniso} &= 0.0867 \\ \bar{E} &= 664.17 \text{ MPa} \\ sd(E) &= 21.34 \text{ MPa} \\ \bar{G} &= 276.04 \text{ MPa} \\ sd(G) &= 33.70 \text{ MPa} \end{aligned}$$

$$\mathbb{C}_{\substack{n=9 \\ N=5}} = \begin{bmatrix} 799.63 & 265.22 & 268.71 & -10.46 & -8.25 & -2.03 \\ & 812.57 & 265.94 & -0.71 & -1.24 & -2.42 \\ & & 804.82 & 7.5 & 11.44 & 4.11 \\ & & & 273.90 & -1.8 & -1.58 \\ & \text{Sym.} & & & 275.48 & 1.75 \\ & & & & & 279.83 \end{bmatrix} \text{ MPa}$$

$$\begin{aligned} \bar{E}_P &= 681.64 \text{ MPa} \\ \bar{G}_P &= 273.65 \text{ MPa} \\ \kappa_{aniso} &= 0.0249 \\ \bar{E} &= 668.79 \text{ MPa} \\ sd(E) &= 33.72 \text{ MPa} \\ \bar{G} &= 274.9 \text{ MPa} \\ sd(G) &= 23.38 \text{ MPa} \end{aligned}$$

$$\mathbb{C}_{\substack{n=9 \\ N=15}} = \begin{bmatrix} 808.67 & 259.27 & 268.68 & -2.24 & -0.18 & -4.84 \\ & 818.4 & 260.38 & 1.87 & -2.04 & -4.88 \\ & & 812.38 & -0.65 & 3.25 & 6.50 \\ & & & 273.53 & -6.43 & -1.53 \\ & \text{Sym.} & & & 275.84 & -3.97 \\ & & & & & 273.97 \end{bmatrix} \text{ MPa}$$

$$\begin{aligned} \bar{E}_P &= 683.87 \text{ MPa} \\ \bar{G}_P &= 274.74 \text{ MPa} \\ \kappa_{aniso} &= 0.0182 \\ \bar{E} &= 680.12 \text{ MPa} \\ sd(E) &= 39.8 \text{ MPa} \\ \bar{G} &= 272.62 \text{ MPa} \\ sd(G) &= 20.42 \text{ MPa} \end{aligned}$$

$$\mathbb{C}_{\substack{n=9 \\ N=30}} = \begin{bmatrix} 809.61 & 256.54 & 269.77 & -0.85 & 2.29 & -1.7 \\ & 820.48 & 264.18 & 0.67 & -0.67 & -3 \\ & & 806.3 & -0.23 & 0.65 & 1.16 \\ & & & 270.51 & -2.75 & -1.08 \\ & \text{Sym.} & & & 278.13 & -2.16 \\ & & & & & 276.12 \end{bmatrix} \text{ MPa}$$

$$\begin{aligned} \bar{E}_P &= 683.78 \text{ MPa} \\ \bar{G}_P &= 274.68 \text{ MPa} \\ \kappa_{aniso} &= 0.0135 \\ \bar{E} &= 678.38 \text{ MPa} \\ sd(E) &= 43.35 \text{ MPa} \\ \bar{G} &= 273.1 \text{ MPa} \\ sd(G) &= 19.78 \text{ MPa} \end{aligned}$$

One can see $\mathbb{C}$ gradually obtaining isotropic shape for an increasing number of samples. This is quantified by the decreasing degree of anisotropy. Due to the small differences between $N = 15$ and $N = 30$ realisations it is concluded that using $N = 15$ throughout the present study is reasonable.

Furthermore, the hypothesis of ergodicity states that averaging a mechanical field at a fixed point over all possible realisations (the ensemble) yields the same result as averaging over the volume of one infinitely large sample. This is a pivotal assumption in computational homogenisation, as the time complexity of solving the system of equations is $O(n^3)$, via Gauss-Seidel. Furthermore, RVE sizes are often limited by the available RAM. The following results for $n = 50$ and $n = 100$ indicate that using large samples yields approximately the same results as a high number of small samples.

$$\begin{aligned}
 \mathbb{C}_{n=50}^{N=1} &= \begin{bmatrix} 827.56 & 255.98 & 250.95 & -0.37 & -2.15 & -5.90 \\ & 808.87 & 263.12 & -3.35 & -4.02 & -10.61 \\ & & 838.26 & 3.68 & -3.07 & 10.06 \\ & & & 271.74 & -5.42 & -3.02 \\ & \text{Sym.} & & & 271.72 & 3.49 \\ & & & & & 273.10 \end{bmatrix} \text{ MPa} \\
 &\quad \begin{aligned} \bar{E}_P &= 688.40 \text{ MPa} \\ \bar{G}_P &= 276.96 \text{ MPa} \\ \kappa_{aniso} &= 0.0295 \\ \bar{E} &= 691.72 \text{ MPa} \\ sd(E) &= 16.18 \text{ MPa} \\ \bar{G} &= 272.41 \text{ MPa} \\ sd(G) &= 0.6 \text{ MPa} \end{aligned} \\
 \\
 \mathbb{C}_{n=100}^{N=1} &= \begin{bmatrix} 817.58 & 249.51 & 269.29 & 2.55 & -4.67 & -5.39 \\ & 821.94 & 258.91 & -6.93 & 3.46 & 10.34 \\ & & 812.70 & 3.36 & 3.31 & -8.25 \\ & & & 264.00 & -7.32 & 1.51 \\ & \text{Sym.} & & & 281.00 & 3.59 \\ & & & & & 273.28 \end{bmatrix} \text{ MPa} \\
 &\quad \begin{aligned} \bar{E}_P &= 684.76 \text{ MPa} \\ \bar{G}_P &= 275.29 \text{ MPa} \\ \kappa_{aniso} &= 0.0302 \\ \bar{E} &= 702.41 \text{ MPa} \\ sd(E) &= 10 \text{ MPa} \\ \bar{G} &= 271.9 \text{ MPa} \\ sd(G) &= 8.5 \text{ MPa} \end{aligned}
 \end{aligned}$$

2.5.2 Definition of a Qualitative Measure of Convergence

The RVE is defined as the smallest volume of heterogeneous material that captures the global — i.e. smeared — properties. Real or virtual testing of smaller than representative volumes will introduce errors to the results, since microstructural fluctuations have not yet averaged out. The required size is dependent on the morphological or physical property of investigation. Furthermore, Kanit et al. [96] point out, that it is also possible to make use of ergodicity by using a high number of realisations for not converged RVE sizes to obtain apparent properties with high accuracy. However, this procedure is not valid for arbitrary small RVEs since one has to make sure that the mean is not biased. Furthermore, the material contrast demands the use of PBCs in order to rule out the influence of boundary conditions on the RVE size.

The methodology adopted here is employed by various researchers to provide a qualitative measure of n [96; 162; 67]. Throughout this work, n is chosen as a multiple of 3. By assuming that the homogenised material response is normally distributed, we define a property as converged, if we can be $2sd \triangleq 95.45\%$ confident, that a random sample is not further away from the expectancy than 7%. In other words, the double of the coefficient of variation, c_v , has to become

$$2c_v(E) = \frac{2sd(E)}{\bar{E}} < 0.07. \quad (2.18)$$

$2c_v(G)$ is defined analogously. A monotonuos evolution of c_v cannot be expected for practical values of n & N . Thus, it is additionally required that $2c_v < 0.07$ holds for three consecutive choices of n in order to ensure systematic and rule out accidental convergence. For the material contrasts up to 1000 investigated here, a $2sd$ confidence interval and a threshold of 7% seem reasonable and furthermore do not restrict the generality of the method.

2.6 Results & Discussion

Here, qualitative bounds for the minimal RVE size are obtained for linear elastic mechanical properties of the composite. In section 2.6.1, the influence of c_{RM} is investigated for three different c_{RM} spanning two orders of magnitude. Φ_R is kept constant at 0.63. Asphalt types vary in terms of bitumen content, pores, additives and their granulometric curve. In order to take this variability into account, required RVE sizes are determined numerically for five values of Φ_R in section 2.6.2. All errorbars show $2sd$ confidence intervals. Numerical values show 4 significant digits for reasons of lucid presentation.

2.6.1 Influence of Material Contrast

Immediate convergence with no influence of Φ_R , or n , is obtained for setting c_{RM} to unity, which corresponds to homogeneous material. The same holds for setting Φ_R to zero, or unity. These extreme cases of c_{RM} and Φ_R rule out the influence from the morphology. It is expected that an increase of the material contrast, c_{RM} , yields larger RVEs since strain and stress heterogeneities grow. In order to obtain a result that is independent of the drawn samples, the three sets of computations for the investigation of the influence of c_{RM} share the same geometries. Hence, a similar shape of the graphs is obtained.

The behaviour of the three Young's moduli for $c_{RM} = 1000$ with increasing n is shown in figure 2.9. figure 2.10 shows the results for the shear moduli. It can be seen that the mean moduli exhibit very little fluctuation with a small bias only for very coarse structures. Furthermore, the statistical scatter reduces rather slowly. This is in

	$c_{RM} = 10$	$c_{RM} = 100$	$c_{RM} = 1000$
$\bar{E}$ [MPa]	$2.74 \times 10^4 \pm 1039$	4280 ± 268.4	452.1 ± 24.3
$\bar{G}$ [MPa]	$1.1 \times 10^4 \pm 470.2$	1672 ± 113.3	179.5 ± 10.06

Table 2.3: Homogenised material properties, $\bar{E}$, $\bar{G}$, and their double standard deviation, for a variation of the material contrast spanning two orders of magnitude. Φ_R is fixed to 0.63.

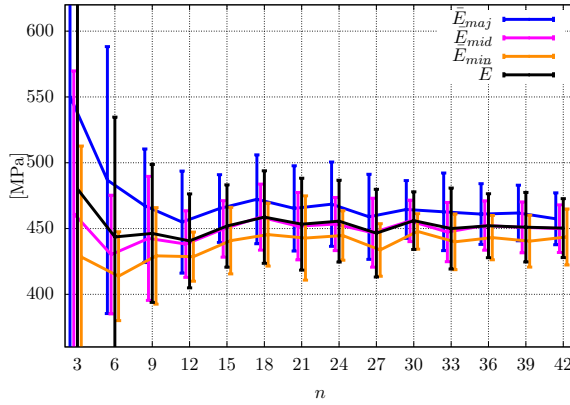


Figure 2.9: Young's moduli for different numbers of seeds n . $\Phi_R = 0.63$ and $c_{RM} = 1000$.

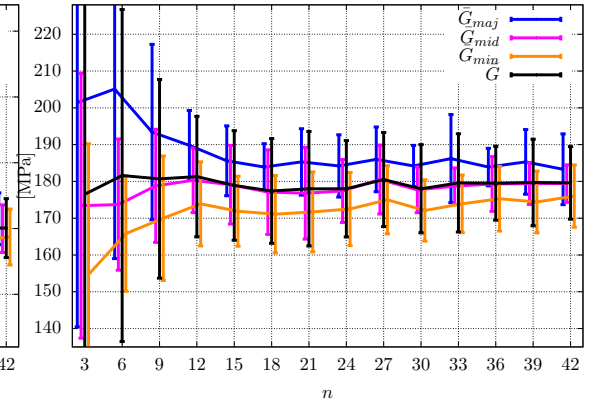


Figure 2.10: Shear moduli for different numbers of seeds n . $\Phi_R = 0.63$ and $c_{RM}=1000$.

agreement with the findings of Kanit et al. [96] for a polycrystalline metal structure. They attribute the latter to the use of PBCs.

As E_R is kept constant, decreasing c_{RM} corresponds to increasing the mortar stiffness. The drastic influence of the mortar phase on the RVE size can be inferred from the double coefficients of variation $2c_v(\bar{E}, c_{RM})$ and $2c_v(\bar{G}, c_{RM})$ given in figure 2.11 and figure 2.12. Numerical values are given in table 2.5. By changing the mortar stiffness from 80 to 800 MPa, an almost tenfold increase in $\bar{E}$ is observed. The effect slightly wears out with increasing E_M further to 8000 MPa; $\bar{E}$ grows approximately sixfold. See table 2.3 for the homogenised material properties.

It is concluded that computing 15 realisations per value of n is sufficient to highlight the influence of c_{RM} , since lower contrasts strictly yield lower n . Lowering c_{RM} from 1000 to 100 yields the same drastic reduction of n by four increments of 3 as a further decrease of the contrast to $c_{RM} = 10$. As expected, an increase of c_{RM} requires larger RVE sizes.

	$\Phi_R = 0.33$	$\Phi_R = 0.43$	$\Phi_R = 0.53$	$\Phi_R = 0.63$	$\Phi_R = 0.73$
$\bar{E}$ [MPa]	182.9 ± 8.232	239.9 ± 15.66	323.3 ± 20.74	452.1 ± 24.3	676.1 ± 40.04
$\bar{G}$ [MPa]	69.49 ± 3.96	92.19 ± 5.614	126 ± 8.138	179.5 ± 10.06	274 ± 18.23

Table 2.4: Homogenised material properties $\bar{E}$, $\bar{G}$, and their double standard deviation for a fixed material contrast of $c_{RM}=1000$ and five different volume fractions.

2.6.2 Influence of Volume Fraction

As previously mentioned, immediate convergence is achieved for setting $\Phi_R = 0$ as well as for setting $\Phi_R = 1$. High values of c_{RM} amplify the differences between different choices of Φ_R . Thus, $c_{RM} = 1000$ is used here in order to highlight these differences.

The influence of Φ_R for fixed c_{RM} on the RVE size can be inferred from figure 2.13 and figure 2.14. No significant change in RVE size is seen when Φ_R is decreased from 0.73 to 0.63, see also table 2.5. However, when Φ_R is further decreased, smaller values of n are sufficient. The present data indicate an increase in RVE size with increasing Φ_R . The homogenised material properties are given in table 2.4. There, it can clearly be seen that the homogenised stiffnesses are dominated by the mortar properties.

2.6.3 General Findings

The values for $c_v(\bar{E})$ and $c_v(\bar{G})$ are given in table 2.5. No clear statement can be given whether E or G converges faster. In general, it can be said that the mean middle moduli obtained from $\mathbb{C}$ provide a good estimate of the overall mean values: $\bar{E} \approx \bar{E}_o$ and $\bar{G} \approx \bar{G}_o$. Furthermore, the respective mean major and mean minor moduli are approximately equidistant to the mean middle and thus overall mean modulus. c_v , as defined by (2.18), can also be interpreted as a measure of isotropy. Thus, isotropic behaviour of the composite asphalt is also provided in the same statistical sense.

2.7 Summary & Conclusions

In this work, the influences of the material contrast and volume fraction on the size of linear elastic RVEs of geometric models of asphalt based on shrunk Poisson Voronoi tessellations have been determined numerically. For the parameter sets investigated here, RVE sizes range from $n = 12$ in the best cases, to $n = 36$ in the worst cases, see table 2.5.

The results clearly show that higher material contrasts require larger RVEs. This finding is of particular importance for temperature dependent materials as asphalt. RVE dimensions must not only be determined for one arbitrary temperature, but for

the worst case, i.e. the one showing the highest contrast. However, the simplification to linear elastic materials has to be kept in mind here. The incorporation of further heterogeneities should yield larger RVEs and strain localisations caused by inelastic material behaviour are undoubtedly increasing heterogeneity. Nevertheless, particularly the incorporation of viscoplastic behaviour relaxes stress concentrations. In this case, the strain field becomes more heterogeneous, but the stress field does the opposite. Inelastic modelling of the mortar is a currently undertaken extension of the model and will shed light on this subject.

The influence of Φ_R is equally striking. Increasing volume fractions of the reinforcing rock phase monotonously lead to larger RVEs. Performing the following thought experiment supports the findings. Starting from $\Phi_R = 0$ and increasing it, grains grow in size, gain more and more influence on the effective properties, and increase e.g. strain heterogeneity. In the case of a shrunk Voronoi tessellation, the layer thickness between grains tends to zero as Φ_R approaches unity. For a material contrast that is high enough for the strains to dominantly localise in the mortar, the application of arbitrarily small global strains will cause the local strains to grow over all bounds. As $\Phi_R = 1$ is reached, the material is homogeneous again and no localisations occur. Thus, it is hypothesised that there is a singularity for the size of linear elastic RVEs for high c_{RM} :

$$\lim_{\Phi_R \rightarrow 1} n = \infty, \forall c_{RM} \gg 1. \quad (2.19)$$

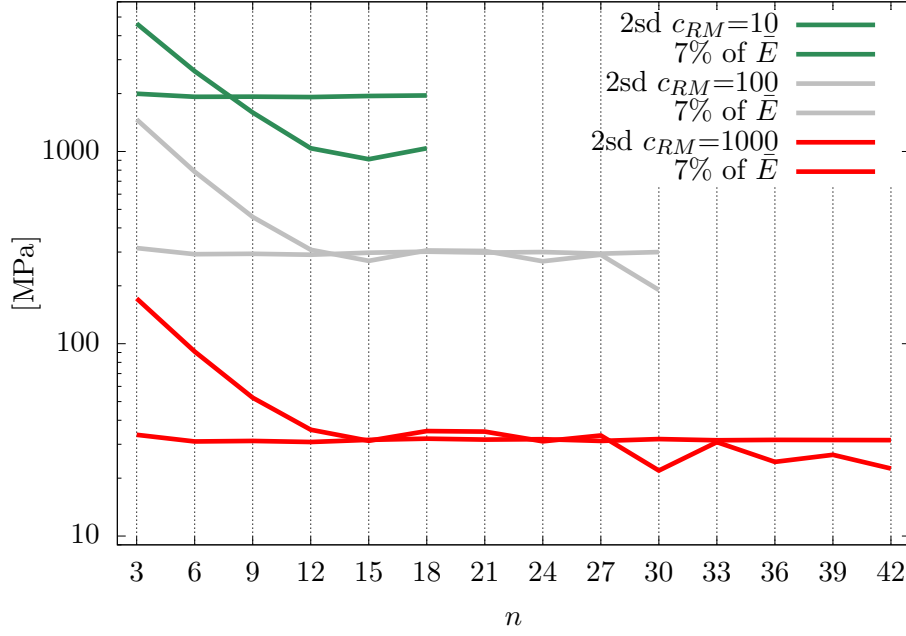
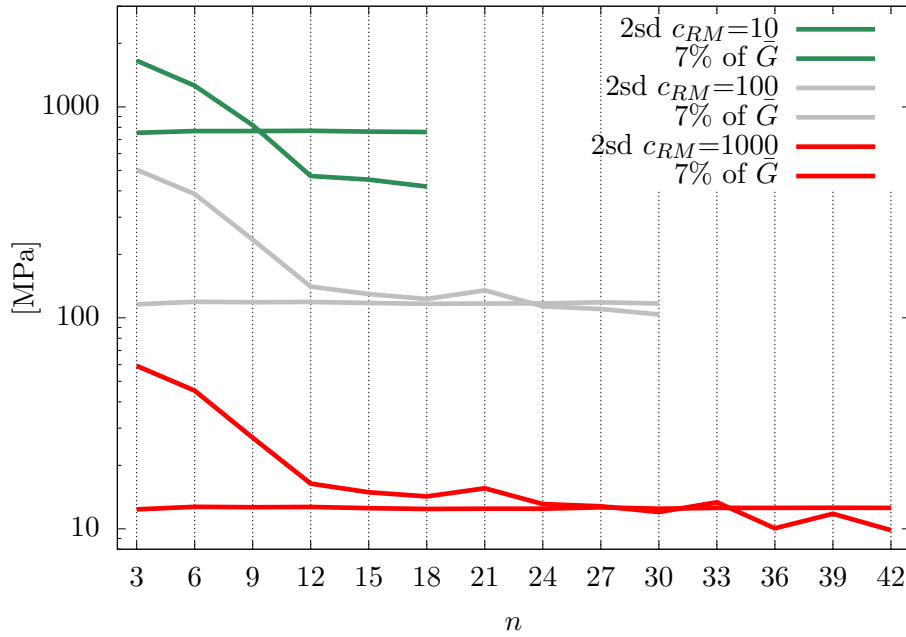
This case is not only of theoretical interest, although $\Phi \rightarrow 1$ is not realistic for most materials. The local layer thickness between adjacent reinforcing grains, particles, or fibres can approach zero (cf. figure 2.1) and strain and stress concentrations will occur at least for elastic materials. In the present model of asphalt, this could be achieved by a rotation of the grains. Furthermore, particular attention is necessary for materials that do not exhibit constant values of Φ due to phase changes, chemical reactions, etc.

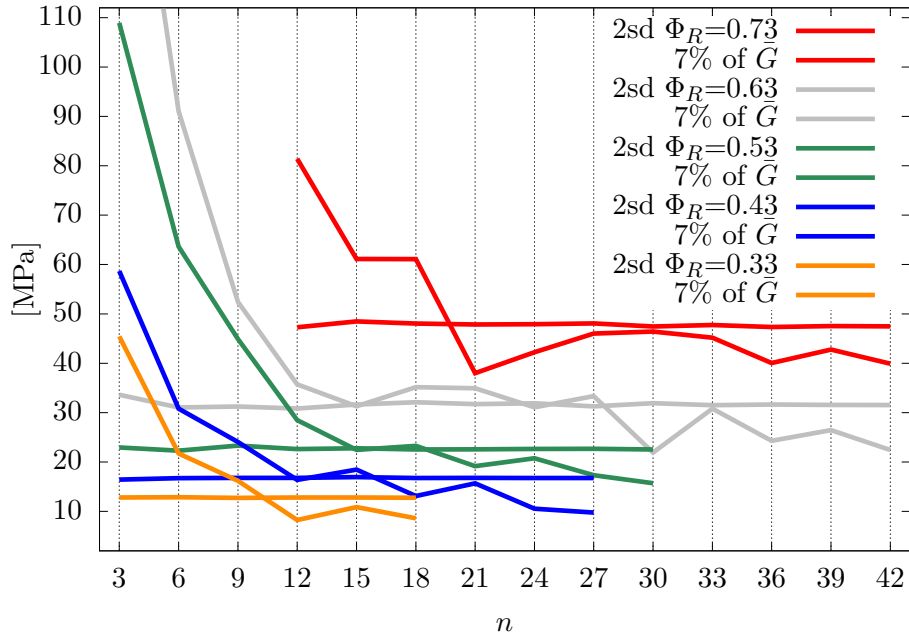
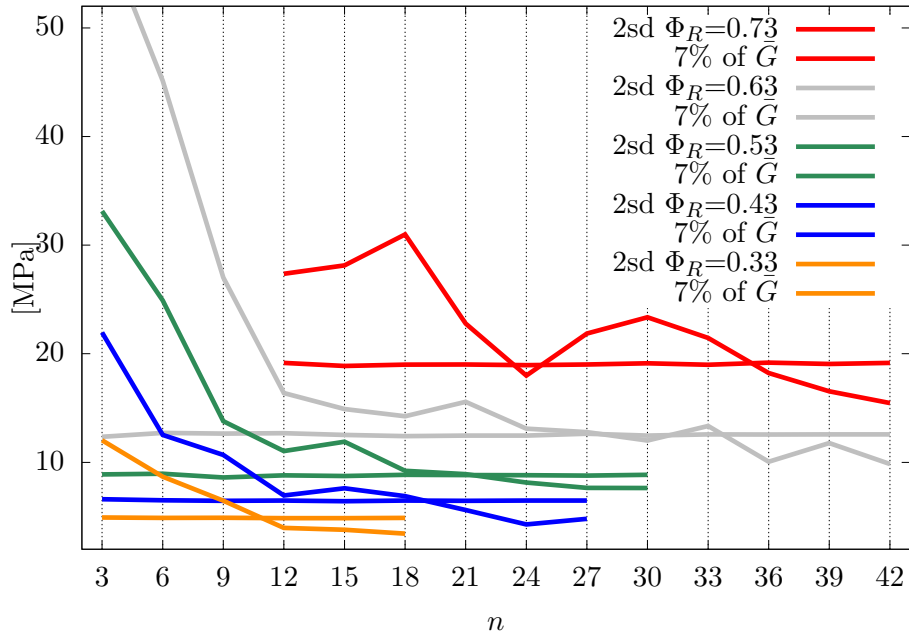
In general, the recommendation to perform worst case oriented RVE design can be given to the practitioner. For the idealised model of asphalt in the present study, the worst case are high values of both c_{RM} and Φ_R . The impressions gained from corresponding literature support the generalisation that increasing the material contrast means increasing the RVE size. Unfortunately, no clear picture can be drawn for the volume fraction. E.g. Stroeven et al. [162] conclude that “... *lower* [particle – author’s note] *densities generally lead to larger RVEs*”, which seems contradictory to the present findings.

Acknowledgements

The authors gratefully acknowledge the financial support of the German Federal Highway Research Institute (BAST) by research grant FE 07.0264/2012/ARB. Furthermore, the authors want to express their gratitude towards the anonymous reviewers

for the constructive criticism which helped to improve the quality of this work. Finally, J.Wimmer likes to thank Mauricio Lobos for the discussion about isotropic projectors.

Figure 2.11: $2c_v(E)$ with increasing n for $\Phi_R = 0.63$ and all c_{RM} .Figure 2.12: $2c_v(G)$ with increasing n for $\Phi_R = 0.63$ and all c_{RM} .

Figure 2.13: $2c_v(E)$ with increasing n for $c_{RM}=1000$ and all Φ_R .Figure 2.14: $2c_v(G)$ with increasing n for $c_{RM}=1000$ and all Φ_R .

n	$2c_v$ [%]					
	$\Phi_R = 0.33$		$\Phi_R = 0.43$		$\Phi_R = 0.53$	
	$c_{RM} = 1000$	$c_{RM} = 1000$	$c_{RM} = 1000$	$c_{RM} = 1000$	$c_{RM} = 10$	$c_{RM} = 100$
3	24.84, 17.14	25.01, 23.27	33.23, 26.09	16.22, 15.39	32.63, 30.41	35.8, 33.54
6	11.83, 12.43	12.89, 13.47	19.98, 19.48	9.515, 11.47	18.77, 22.71	20.53, 24.86
9	8.901, 9.237	10.04, 11.57	13.48, 11.22	5.784, 7.466	10.86, 13.84	11.75, 14.95
12	4.5, 5.699	6.834, 7.505	8.81, 8.781	3.793, 4.276	7.429, 8.277	8.109, 9.035
15	5.93, 5.457	7.62, 8.294	6.903, 9.523	3.286, 4.144	6.347, 7.716	6.919, 8.334
18	4.724, 4.929	5.478, 7.438	7.226, 7.293	3.723, 3.854	7.091, 7.375	7.663, 8.03
21		6.527, 6.09	5.946, 7.069		7.132, 8.083	7.709, 8.747
24		4.405, 4.623	6.418, 6.462		6.272, 6.779	6.823, 7.362
27		4.081, 5.178	5.352, 6.1		6.915, 6.509	7.466, 7.086
30			4.877, 6.038		4.449, 6.211	4.807, 6.743
33						6.845, 7.434
36						5.372, 5.604
39						5.862, 6.556
42						4.983, 5.486

Table 2.5: Double coefficient of variation in percent. $c_v(\bar{E})$ in front of comma, $c_v(\bar{G})$ after. Paired values which fulfill the convergence criterion are in bold.

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

This article was published as:

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J. Neumann devised and implemented the geometry model generation in **Matlab**, fit the generalised Maxwell model to the data, ran the simulations, interpreted the data, and wrote the major part of the article.

K. Mollenhauer performed the DSR experiments on bituminous mortar, constructed the master-curve from data, and took part in writing the article.

J.-W. Simon and S. Reese provided intellectual content and gave conceptual advice.

S. Reese was engaged in obtaining funds for the research.

All authors drafted the work for intellectual content.

All authors approved the publication of the final manuscript.

3.1 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.

3.2 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 NMAS [149]. Furthermore, the material contrast between the constituents is known to influence the variability of mechanical response and therefore representativeness, see e.g. [141; 178]. 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 [178] 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 mortar¹ phase is assumed, which consists of bitumen and aggregates smaller than the threshold, see figure 3.1 for an illustration of the scale separation used here. A threshold of 2 mm is a natural choice for PSDs based on the metric system [26; 179; 59; 93]. The cumulative mass percentage of passing aggregates at this sieve size is always given by German standards [65; 22]. Consequential, dynamic shear rheometry according to DIN EN 14770 [6] for testing pure bitumen cannot be applied to measure the properties of the viscoelastic mortar phase using standard 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 3.3.

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 Caro et al. [44]; Wang and Hao [174]; Aragão et al. [32]; Karki et al. [98]; Ozer et al. [141]. These models require only moderate computational resources, but it has been shown that 2D modelling is often not valid. Fakhari Tehrani et al. [59] 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 [127; 47; 46; 141]. 3D models typically rely on XRCT scanned samples, see e.g. the works of Kutay et al. [105]; Coleri et al. [47]; You et al. [184]; Schüller et al. [157]. Image based modelling requires that the geometry, which is to be modelled, has to exist *a priori*. However,

¹Also termed Fine Aggregate Matrix (FAM) in the corresponding literature.

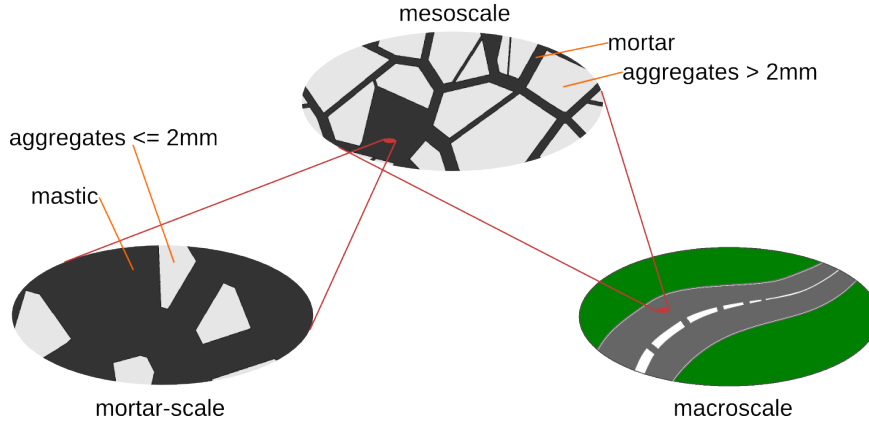


Figure 3.1: Scale separation within asphalt used here.

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 [127; 92; 156], or polygons [100; 192; 102; 175; 50]. 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 [125]. However, the accuracy of the aggregate shapes is critical, as Yang et al. [183] emphasise in a review article about heterogeneous modelling efforts of stone based materials.

Only a few synthetic 3D geometry generators for the finite element method² have been reported. Mo et al. [127] developed a monodisperse sphere model for ravelling analysis of porous asphalt. Dai [51] also used a monodisperse sphere model with damage modelling to compute indirect tension and compression experiments on virtual samples. Fakhari Tehrani et al. [59] 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 [60]. A similar path is followed by Cao et al. [43], who used a 3D compaction simulation but moduli predictions were executed in 2D. Chen et al. [46] used extruded polygons, which are not strictly convex. They presented parameter studies of aggregate orientation as well as air void distribution and size. Schüller et al. [157] 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 random³ VT and then iteratively retessellates (thus nested tessellation) aggregates

²Generators for the discrete element method are not considered here.

³The peculiarities of pseudorandom number generation are out of scope of this paper. Hence “pseudo” is dropped for reasons of brevity.

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. Nygård and Gudmundson [137]. 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 3.4.

Among the boundary conditions that satisfy the Hill-Mandel condition, periodic displacement boundary conditions are the preferred choice in order to establish minimally sized RVEs. The response under displacement based PBCs 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 [88]; Huet [89]; Miehe [124]; Ostoja-Starzewski [140]; Saeb et al. [152]. Based on these theoretical findings, several authors predicted the macroscale response of viscoelastic composites using computational homogenisation, see e.g. Schüller et al. [156]; Zhang and Ostoja-Starzewski [187]; Schüller et al. [157]; Zhang and Ostoja-Starzewski [188]. PBCs require periodicity of geometry and mesh at the domain boundary. Periodic random VTs are generated using seed periodisation, see e.g. Decker and Jeulin [54]; Fritzen and Böhlke [67]; Wimmer et al. [178]. 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. Schüller et al. [157]. 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 3.5.

Numerical results of the homogenised mechanical properties of German standard type stone mastic asphalt (SMA 8 S) are presented in section 3.6. The required domain volume for a statistical requirement of representativeness is given. Furthermore, the effect of reinforcement is analysed in mono- and polydisperse samples and differences are highlighted. Finally, the influence of the loading rate on material contrast and thus the scatter in the homogenised response is investigated.

3.3 Material Characterisation

This section presents the experimental procedure for the bituminous mortar. Following Huurman and Mo [91], oscillatory shear tests are conducted to yield viscoelastic data over a large frequency and temperature range. The time-temperature superposition is

employed to construct master-curves. Subsequently, the generalised Maxwell model is fit to the data using Tikhonov regularisation.

3.3.1 Experimental Procedure

The bituminous mortar phase of a German standard HMA was prepared at the Institute of Highway Engineering Aachen. The HMA composition represents that of stone mastic asphalt (SMA 11 S) according to DIN EN 13108-5 [22], targeting a mix level air void content of 2.8 v.%. The mix consisted of 6.7 m.% polymer modified bitumen PmB 25/55-55A, 0.3 m.% cellulose fibres, limestone filler, crushed sand and stone both made of diabase. The mortar was then produced by *not* adding the mineral aggregate fractions > 2 mm. This resulted in the pure mortar composition given in table 3.1. Based on this procedure, the mortar is assumed to be free of pores. This mortar design neglects that the aggregates adsorb some of the bitumen which results in a thin film between aggregates and mortar that is believed to be a few μm thick [146; 172]. This has two important consequences. First, bitumen is overdosed in the mortar tested here. Second, the effective properties of one and the same mortar change once it is mixed with the larger aggregate fractions of differently graded asphalt types due to different surface areas. However, these effects are not a subject of the present investigation. Karki et al. [98] and Im et al. [95] both reduced the bitumen content of their mortars to values below what was dictated by mix level.

	PmB	fibres	filler < 0.063 mm	sand (0.063 to 1 mm)	sand (1 to 2 mm)
m.%	21.1	1	30.6	34.7	12.6

Table 3.1: Mortar composition.

The mortar was cast into cylindrical silicone moulds with a diameter of 5 mm and 10 mm height, see figure 3.2. After solidification and removal from the moulds, the specimens were subjected to oscillating torsional loading in an **Anton Paar MCR 302** solid state rheometer, see figure 3.3. The oscillation tests have been performed at a shear strain amplitude of 0.1%, for which response in the linear viscoelastic regime has been confirmed by running amplitude sweep tests at lowest temperature/highest frequency and highest temperature/lowest frequency according to DIN EN 14770 [6]. The frequency range was chosen in ten steps between $0.01 \text{ Hz} \leq f = \omega/(2\pi) \leq 10 \text{ Hz}$. The temperature was varied as follows: 40°C , 30°C , 20°C , 10°C , 0°C , -10°C , -20°C and 40°C (in order to rule out specimen damage), and finally 50°C . The cylindrical mortar specimens used here are relatively small in comparison to samples used by other researchers. Woldekidan et al. [179] used cylinders of 12×6 mm (height $\times$ diameter) together with a mortar that contained aggregates up to 2 mm. Later, the same group used cylinders with a slightly shorter free length of 10 mm for a mortar that contained

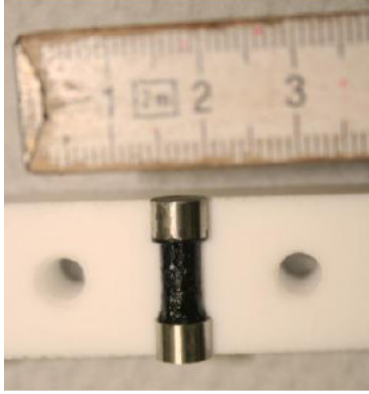


Figure 3.2: Cylindrical specimen of SMA mortar.

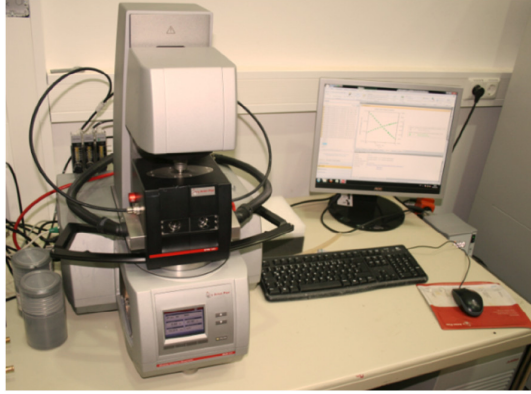


Figure 3.3: Left: Overview of the rheometer setup. Right: Closeup of the specimen in the testing device.

only fine aggregates up to 0.5 mm [180]. Karki et al. [98]; Im et al. [95] used cylinders of dimensions 45×12.25 mm for a mortar that contained sand ≤ 1.18 mm. A systematic determination of representative sample size has not been undertaken at this point. Three samples have been tested and there is scatter, as can be seen in figure 3.7. Interestingly, the scatter is more pronounced in the low frequency/high temperature regime, which is in agreement with later presented findings, c.f. section 3.6.3. In road materials testing, a ratio of largest aggregate size to the lowest test sample dimension shall be higher than 3. Here, only 4 m.% of the grains within the mortar sample have a grain diameter larger than $\frac{5}{3} \approx 1.7$ mm which allows cautious optimism that the samples are representative. Since these types of experiments become more common, a thorough experimental investigation of representative sample size is necessary, which could be aided by numerical simulations in a similar way to the presented one. The testing procedure yields the complex shear modulus, G^* , and the loss angle, δ . The following relations apply:

$$G^* = G' + iG'' , \text{ and } \tan \delta = \frac{G''}{G'} , \quad (3.1)$$

where G' , G'' , and i are the storage modulus, the loss modulus and the imaginary unit, respectively. For reasons of simplicity, the absolute value of G^* , $|G^*|$, is used which is the ratio of shear stress amplitude, τ_0 , over shear strain amplitude, γ_0 :

$$|G^*| = \frac{\tau_0}{\gamma_0} = \sqrt{(G'^2 + G''^2)} . \quad (3.2)$$

Displaying the data of a single sample in Black (see figure 3.4) and Cole-Cole (see figure 3.5) plots show that a continuous curve can be drawn through the data points,

with small deviations for 50 °C. This indicates the validity of the time-temperature superposition principle. Consequently, an Arrhenius-type shift function is employed to construct master-curve data for a reference temperature, T_{ref} , of 20 °C. This results in a reduced frequency range of 1×10^{-4} Hz to 1×10^4 Hz. The raw shifted master-curve data of all three samples can be seen in figure 3.7.

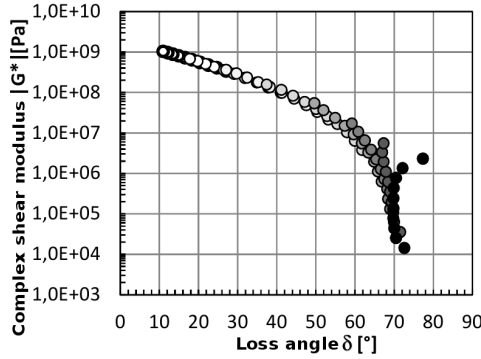


Figure 3.4: Black plot of complex shear modulus versus loss angle of SMA mortar.

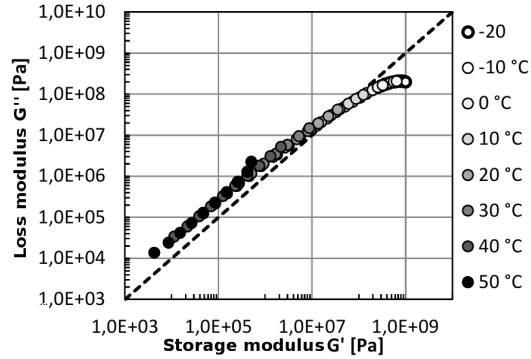


Figure 3.5: Cole-Cole plot of the loss modulus versus storage modulus of SMA mortar.

3.3.2 Model Calibration

The generalised Maxwell⁴ model is widely employed to capture relaxation phenomena that occur on different time scales. It overcomes the narrow bandwidth of a single Maxwell element by arranging an arbitrary number of them in parallel. The interested reader is referred to a review article by Yusoff et al. [185] for an overview of models typically applied to bituminous materials. In order to establish a discrete response function in the time domain, represented through a Prony series, the relaxation function is converted to the frequency domain, where the experiments have been performed. In order to obtain a good fit of the model to the data, it is common practice to have 1–2 Maxwell elements per decade of frequency. Here, the reduced frequency data covers about 8 decades, resulting in a high number of parameters which have to be identified. In general, this constitutes a nonlinear inverse problem which suffers from bad conditioning and noisy data.

Schapery's well-known collocation scheme [154] is used in conjunction with Tikhonov regularisation in order to overcome the previously mentioned problems. In the context of road engineering materials, the groups of Zhu et al. [191], and Ebrahimi et al. [57]

⁴Also termed Maxwell-Wiechert

used Tikhonov regularisation based on the L-Curve in order to fit to data from static creep tests.

The generalised Maxwell model features a discrete relaxation spectrum with $2n + 1$ parameters, where n is the number of Maxwell elements. The storage and loss moduli, G' , and G'' , can be written as

$$G'(\omega) = g_\infty + \sum_{i=1}^n g_i \frac{(\omega\tau_i)^2}{1 + (\omega\tau_i)^2} , \quad (3.3)$$

$$G''(\omega) = \sum_{i=1}^n g_i \frac{\omega\tau_i}{1 + (\omega\tau_i)^2} . \quad (3.4)$$

If the discrete relaxation times, τ_i , are chosen in a reasonable manner, the remaining unknown parameters, g_∞ and g_i , can be determined via a linear least-squares procedure. In principle, it is possible to use either equation 3.3 or equation 3.4 and determine the vector of unknowns, $\mathbf{g}$, using the data of storage and loss moduli, $\hat{G}'$ or $\hat{G}''$, respectively. However, it is more reasonable to use storage and loss moduli simultaneously in an objective function

$$\sum_{j=1}^m \left[\left(G'(\mathbf{g}, \omega_j) - \hat{G}'_j \right)^2 + \left(G''(\mathbf{g}, \omega_j) - \hat{G}''_j \right)^2 \right] = \min . \quad (3.5a)$$

Cast into matrix notation, equation 3.5a can be rewritten as

$$\|\mathbf{A}\mathbf{g} - \hat{\mathbf{G}}'\|_2^2 + \|\mathbf{B}\mathbf{g} - \hat{\mathbf{G}}''\|_2^2 = \min , \quad (3.5b)$$

with $\hat{\mathbf{G}}'$ and $\hat{\mathbf{G}}''$ being the experimental data of storage and loss moduli in vectorial notation, respectively. Furthermore, the matrices $\mathbf{A}, \mathbf{B} \in \mathbb{R}^{m \times n}$, where m is the number of experimental data pairs, are given as follows:

$$\mathbf{A} = \begin{bmatrix} 1 & \frac{(\omega_1\tau_1)^2}{1+(\omega_1\tau_1)^2} & \cdots & \frac{(\omega_1\tau_n)^2}{1+(\omega_1\tau_n)^2} \\ 1 & \frac{(\omega_2\tau_1)^2}{1+(\omega_2\tau_1)^2} & & \vdots \\ \vdots & & \ddots & \vdots \\ 1 & \frac{(\omega_m\tau_1)^2}{1+(\omega_m\tau_1)^2} & \cdots & \frac{(\omega_m\tau_n)^2}{1+(\omega_m\tau_n)^2} \end{bmatrix} , \quad \mathbf{B} = \begin{bmatrix} 0 & \frac{\omega_1\tau_1}{1+(\omega_1\tau_1)^2} & \cdots & \frac{\omega_1\tau_n}{1+(\omega_1\tau_n)^2} \\ 0 & \frac{\omega_2\tau_1}{1+(\omega_2\tau_1)^2} & & \vdots \\ \vdots & & \ddots & \vdots \\ 0 & \frac{\omega_m\tau_1}{1+(\omega_m\tau_1)^2} & \cdots & \frac{\omega_m\tau_n}{1+(\omega_m\tau_n)^2} \end{bmatrix} . \quad (3.6)$$

These matrices become more and more ill-conditioned with increasing n , which can result in a poor fit or negative material parameters, particularly when the data is noisy. This is usually the case. In order to overcome these problems during parameter identification, the simple and well-known Tikhonov regularisation method is employed,

see e.g. [168; 81]. Deriving equation 3.5 w.r.t. $\mathbf{g}$, the parameters, now depending on λ , are calculated via

$$\mathbf{g}(\lambda) = \left(\mathbf{A}^T \mathbf{A} + \mathbf{B}^T \mathbf{B} + \lambda \mathbf{I} \right)^{-1} \left(\mathbf{A}^T \hat{\mathbf{G}}' + \mathbf{B}^T \hat{\mathbf{G}}'' \right). \quad (3.7)$$

Please note that there exist other methods than to put λ on the main diagonal, e.g. finite difference operators [57]. The regularising parameter λ is determined empirically using the L-Curve [81], which displays the norm of the solution $\|\mathbf{g}(\lambda)\|_2$ as a function of the norm of the residual $\|\mathbf{G}^*(\omega) - \hat{\mathbf{G}}^*\|_2$, see figure 3.6.

The data is lacking a plateau in the low frequency regime, see figure 3.7. Thus, the equilibrium spring with its stiffness g_∞ is neglected and the first columns of $\mathbf{A}$ and $\mathbf{B}$ are omitted. Now, the generalised Maxwell model is representing fluid-like behaviour with permanent deformations. This is supported by the Cole-Cole plot, see figure 3.5, which shows that the loss modulus is dominating over the storage modulus for high temperatures/low frequencies. It is common practice in modelling of bituminous materials to treat the binder as a fluid and the mixture as a solid, see e.g. Oeser and Pellinen [138]. Thus, it can be concluded that the small aggregates present in the mortar do not form a granular skeleton, but are well suspended.

The relaxation times, τ_i , are chosen to be equidistantly spaced on a logarithmic scale. The smallest and largest relaxation times are chosen as $\tau_1 = 0.95 \times \log_{10}(\frac{1}{\omega_{max}})$ and $\tau_n = 0.95 \times \log_{10}(\frac{1}{\omega_{min}})$, respectively. It is found that choosing $n = 10$ provides a small residuum of equation 3.5 and leads to tolerable oscillations of the loss angle, δ . For values of n smaller than 8, oscillations in $|G^*|$ increased drastically. The regularisation parameter, λ , was determined to be 0.37, see figure 3.6. Since a distinct "knee" cannot be seen, λ is chosen as the value that minimises equation 3.5.

The model has been fit to the master-curves of three samples simultaneously in order to take the scatter into account. Thereby, the results are averaged. The final set of parameters is given in table 3.2, while figure 3.7 shows the model fit to the data. The contributions of the individual Maxwell elements to the storage and loss modulus are also depicted. The mineral aggregate consisted of diabase, which is modelled in a linear elastic fashion with a shear modulus of 33.3 GPa and a Poisson's ratio of 0.2. The Poisson's ratio of the mortar has been set to $\nu_M = 0.35$, which is the arithmetic mean between those of pure aggregate and incompressible bitumen.

3.4 Microstructural Modelling of Hot Mix Asphalt

In order to provide a more realistic representation of the microstructure of HMA, several extensions to a previously published version [178] have been undertaken. The most notably one is the representation of the PSD. The proposed method does not require image data, such as XRCT scans, for the microstructure generation and is therefore completely synthetic. The desired PSD is simply provided by the upper and

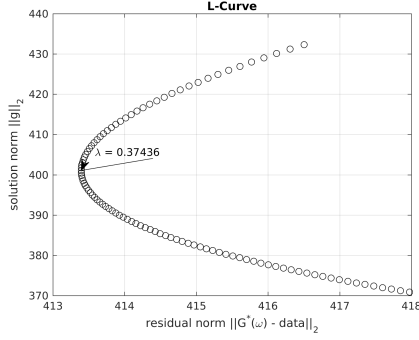


Figure 3.6: L-Curve for the problem equation 3.7 with $0.001 \leq \lambda \leq 1.0$. λ increases from top to bottom.

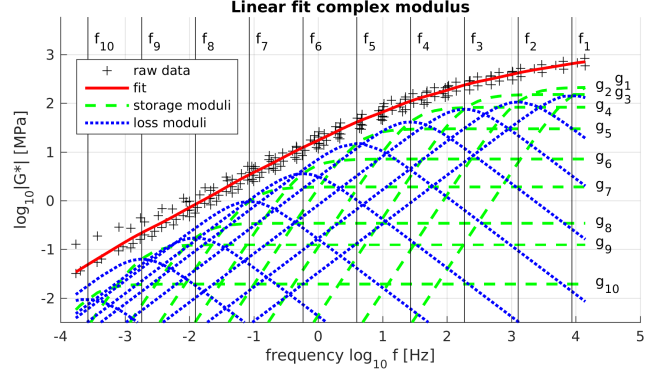


Figure 3.7: Fit.

	$i = 1$	$i = 2$	$i = 3$	$i = 4$	$i = 5$	$i = 6$	$i = 7$	$i = 8$	$i = 9$	$i = 10$
g_i [MPa]	2.92e+2	2.12e+2	1.51e+2	8.28e+1	2.99e+1	7.14e+0	1.91e+0	3.40e-1	1.26e-1	3.43e-2
τ_i [s]	1.15e-4	7.87e-4	5.38e-3	3.68e-2	2.51e-1	1.72e+0	1.17e+1	8.03e+1	5.49e+2	3.75e+3
f_i [Hz]	8.69e+3	1.27e+3	1.86e+2	2.72e+1	3.98e+0	5.82e-1	8.51e-2	1.25e-2	1.82e-3	2.67e-4

Table 3.2: Parameters of the calibrated generalised Maxwell model using 10 parallel elements. The equilibrium modulus has been set to zero, thus a fluid is modelled.

lower bounds for the mass percentage of aggregates passing through the sieve sizes provided by standards, or freely chosen. The algorithm generates a geometry with a discretely modelled target aggregate volume fraction

$$\Phi_A = \frac{V_{A>2mm}}{V_D} \quad (3.8)$$

based on nested Voronoi tessellations. Here, $V_{A>2mm}$ is the volume of aggregates larger than the threshold in a domain volume V_D . In its current form, the algorithm is capable of generating geometries for virtually any type of HMA with isolated voids. However, the voids are not explicitly modelled, which would be unreasonable from a computational point of view. As mentioned previously, a lower threshold of spatial resolution of geometric entities of 2mm is used. Masad et al. [121] investigated the air void distribution in several asphalt specimen using XRCT. In any sample, the median size of air voids was well below this threshold. Although the specific asphalt

type modelled here was not among their investigated samples, it is assumed that well dispersed voids ≤ 2 mm are present.

The geometry generation is implemented in **Matlab**. Extensive use is made of functions provided by the **geom3D** package [113], particularly **minConvexHull**, which is based on **qhull** [36]. In order to obtain the non-convex mortar domain, a wrapper [94] to the **General Polygon Clipper** library [131] is used.

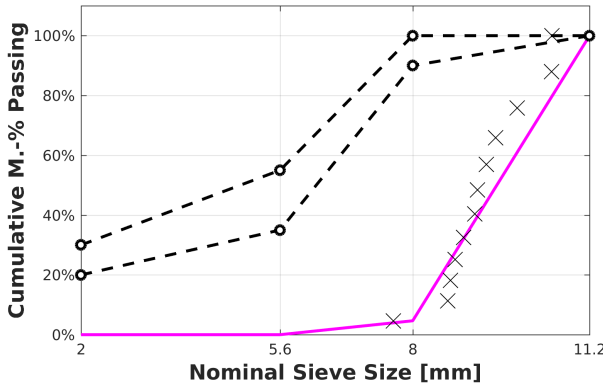
3.4.1 Voronoi Tessellations

A 3D Voronoi tessellation subdivides V_D into non-overlapping volumes V_i that fill V_D . An arbitrary volume V_i is associated with its seed $\mathfrak{s}_i$, such that any point $p \in V_i$ is closer to $\mathfrak{s}_i$, than to any other seed $\mathfrak{s}_j$:

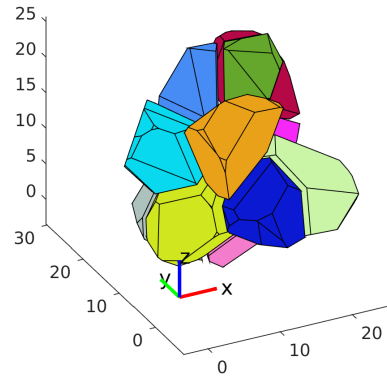
$$V_i = \{p \in V_D | d(p, \mathfrak{s}_i) < d(p, \mathfrak{s}_j), \forall i \neq j\} . \quad (3.9)$$

Here, d is the Euclidean distance, yielding convex polyhedra. Unfortunately, a VT created in that fashion is rather monodisperse and does not follow any typical asphalt PSD, see figure 3.8(a). Such a tessellation will henceforth be called a Pure Voronoi Tessellation (PVT). For reasons of simplicity, the sieve size, S_i , of polyhedron i , is defined to be the diameter of the volume equivalent sphere of V_i :

$$S_i = \sqrt[3]{\frac{6V_i}{\pi}} . \quad (3.10)$$



(a) PSD of PVT with bounds of SMA 8S



(b) View of the PVT

Figure 3.8: The cumulative mass percentage passing of a PVT with $\bar{S} = 9.23 \pm 0.81$ mm is shown in (a). The magenta line indicates the linearisation between discrete sieve sizes. The dashed lines are the upper and lower bounds for the PSD of SMA 8S. A view of the corresponding VT is depicted in (b).

3.4.2 Volumetric Constitution

The densities of bitumen, $\rho_B = 1.05 \text{ g cm}^{-3}$ and diabase $\rho_A = 2.8 \text{ g cm}^{-3}$ allow the computation of Φ_A for a given bitumen content. As mentioned previously, a mass fraction of bitumen of $\chi_B = \frac{m_B}{m_{total}} = 6.7 \text{ m.}\%$ is used here. Furthermore, the influences of voids and filler on the mortar mixture are neglected. Thus, the mixture density, ρ_D , is obtained as

$$\rho_D = \frac{\sum_i m_i}{\sum_i V_i} = \frac{1}{\left(\frac{\chi_B}{\rho_B} + \frac{(1-\chi_B)}{\rho_A}\right)} = 2.52 \text{ g cm}^{-3} . \quad (3.11)$$

The total aggregate volume fraction, Φ_{tA} , which consists of the parts that are geometrically resolved *and* smeared out in the mortar accounts for

$$\Phi_{tA} = \frac{V_A}{V_D} = \frac{m_A}{m_D} \frac{\rho_D}{\rho_A} = (1 - \chi_B) \frac{\rho_D}{\rho_A} = 0.84 . \quad (3.12)$$

With a mean cumulative proportion of aggregates larger than 2 mm of 75 m.%, c.f. figure 3.8(a), and assuming that aggregate mass fractions equal volume fractions, Φ_A can be calculated from the volume of aggregates larger than the threshold, $V_{A>2mm}$, as

$$\Phi_A = \frac{V_{A>2mm}}{V_D} = 0.75 \Phi_{tA} = 0.63 . \quad (3.13)$$

This particular mortar belongs to an SMA 11 S type HMA [65]. Here, the mortar will be used as a representation of a mortar for SMA with 8 mm NMAS as well, although there are small differences between the mixtures with NMAS of 8 and 11 mm. However, this is mainly due to the different surface areas of the asphalt types which are not accurately captured using strictly convex⁵ Voronoi Polyhedra (VPs) anyway.

The domain volume that contains aggregates according to a particular PSD cannot be chosen arbitrarily. Next to mechanical considerations of representativeness, there is an absolute lower bound to the minimum V_D for purely geometrical reasons. Naturally, any sample volume needs to contain at least one aggregate of NMAS. With Φ_{tA} calculated from equation 3.12, and assuming that the mass fraction of aggregates having NMAS equals the volume fraction, $\chi_A^{\text{NMAS}} = \Phi_A^{\text{NMAS}}$, the domain volume can be calculated:

$$V_D = \frac{V_i}{\Phi_A^{\text{NMAS}} \Phi_{tA}} . \quad (3.14)$$

The theoretical minimum domain volume, V_D^{min} , can be computed from the supremum of all possible aggregates having NMAS and the assumption that this aggregate exhausts the lower bound. For SMA 8 S, let's assume that one aggregate that gets just

⁵Among possible other misrepresentations.

retained at 8 mm makes up 10 m.% = v.%, which is the lower bound of the standard, see figure 3.8(a). By solving equation 3.10 for V_i and inserting $S_i^{min} = 8$ mm, one obtains $V_i^{min} > 268 \text{ mm}^3$, thus

$$V_D^{min} > \frac{268 \text{ mm}^3}{0.1 \times 0.84} = 3194 \text{ mm}^3 . \quad (3.15)$$

This is a necessary, but not sufficient bound for SMA 8 S. More reasonable bounds are found when the mean volume of all aggregates with NMAS and the mean volume fraction are inserted into equation 3.14. These values are given in table 3.3. It is usually possible to obtain the PSD within these volumes, indicated by $\bar{V}_D$. Qualitatively similar results in 2D have been found by Romero and Masad [149] based on image analysis of XRCT data.

	S_i^{min} [mm]	V_D^{min} [mm ³]	$\bar{S}$ [mm]	$\bar{V}_D$ [mm ³]
SMA 8 S	> 8	> 3194	9.6	11039
SMA 11 S	> 11.2	> 8765	13.6	31386

Table 3.3: Theoretical minimum and mean values of domain volumes.

Next to the domain volume, also the initial seed density cannot be chosen arbitrarily. Choosing the number of seeds, N , too high will lead to aggregates which are smaller than the maximum aggregate size required by the standard and the PSD can never be matched. N chosen too low will lead to unnecessary retessellation and shrinking steps of the geometry generator and is therefore not economical. Hence, it must be chosen in a way to generate polyhedra with a mean sieve size according to the standard. Using the mean aggregate volume $\bar{V}_A = \Phi_{tA} V_D / N$, equation 3.10 can be solved for the necessary number of seeds employing the floor operator to obtain integers

$$N = \left\lfloor \frac{6 \Phi_{tA} V_D}{\pi \bar{S}^3} \right\rfloor . \quad (3.16)$$

3.4.3 Nested Voronoi Tessellations

One well-known technique to increase the heterogeneity of a VT is the use of weights for the seeds. Schüller et al. [157] proposed to use a particle dynamics approach to create the distribution of weighted seeds. Here, a different method is pursued which relies on nesting the VT. A presumably similar method is implemented in **Neper** [145] from version 3.0.0 onwards. The main idea is to create a Voronoi tessellation within a previously tessellated aggregate. An axis-aligned box is constructed around an aggregate to be retessellated. The centroid of the box coincides with that of the aggregate. The dimensions of the box are twice as large as those of the aggregate. A

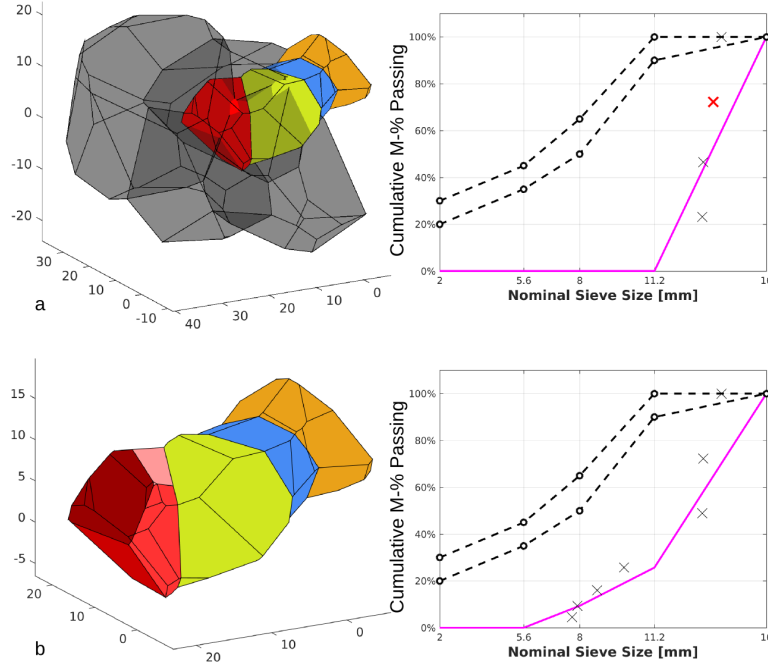


Figure 3.9: Illustration of the nested tessellation. In **a)**, 4 aggregates of a PVT with $\bar{S} = 13.59 \pm 0.39$ mm are depicted on the left, with their cumulative size distribution on the right. The position of the red aggregate is highlighted with a red cross. This aggregate is retessellated into four smaller aggregates by creating the translucent grey aggregates and trimming them to the red one. In **b)**, the resulting smaller aggregates are coloured in different shades of red on the left. On the right, the corresponding PSD is given. Please note that the positions of the two markers which were previously below the red one have changed due to the cumulative nature of the curve.

parameter study showed that putting four seeds inside the box yields useful sizes of the retessellated aggregates. Please refer to figure 3.9 for an illustration of the method.

With the number of seeds for the retessellation carefully chosen to yield reasonably sized smaller aggregates, this nested tessellation can be implemented into an iterative algorithm. A flowchart of this algorithm is depicted in figure 3.10. The algorithm starts with an initial monodisperse VT, whose aggregates' NMAF fits a user-defined standard, also see figure 3.11. The domain volume can be arbitrarily chosen, however, the limits discussed in section 3.4.2 apply. Then, all polyhedra are undergoing a first **shrinking** step. Please note that the initial sieve size had to be compensated for this step, i.e., the initial dense VT had larger aggregates than NMAF *before* shrinking in order to have proper NMAF *after* initial shrinking. The shrinking is carried out

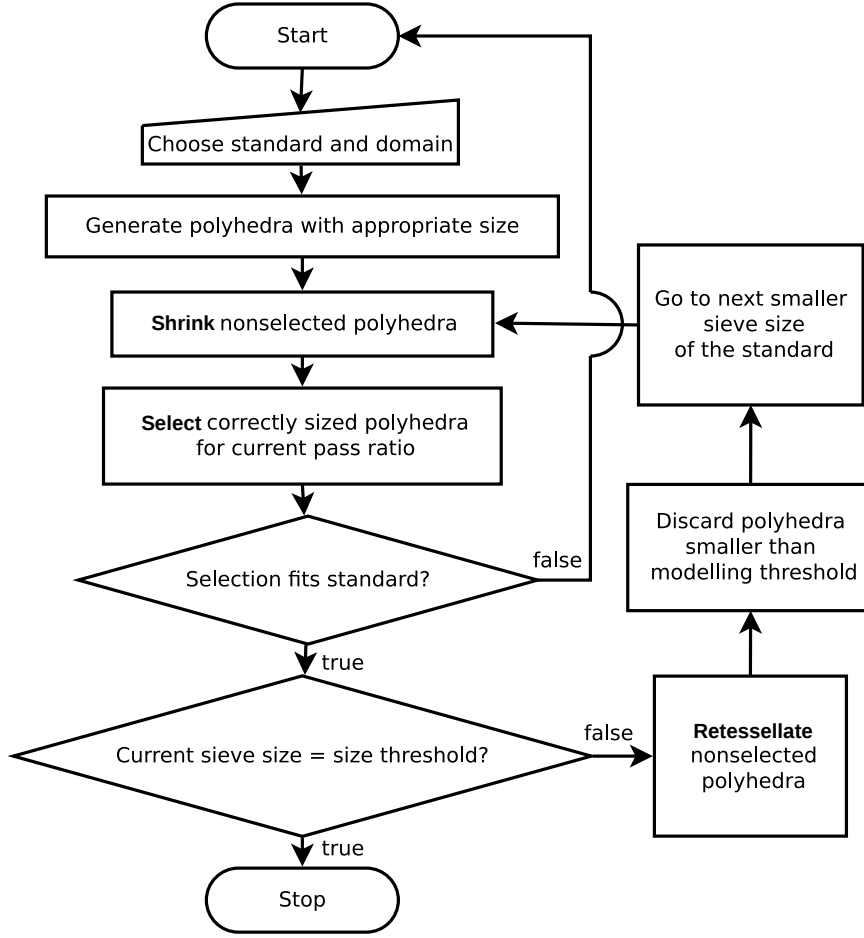


Figure 3.10: Flowchart of the nested Voronoi tessellation algorithm.

towards the centroid of the aggregate. In contrast to shrinking towards the seed, this yields more evenly sized gaps between neighbouring aggregates. For the same reason, the shrinking factor, s , increases with decreasing sieve size. A constant s would lead to narrower gaps as the aggregates become smaller. The shrinking factor is determined using the mean aggregate volume fractions retained at each sieve size S_i , $\bar{\phi}_i$. Again, it is assumed that the mass fractions of aggregates equal their volume fractions. In the next step, aggregates are randomly **selected** from the set of aggregates with current sieve size until the current pass ratio is met⁶. The target is to match the arithmetic mean $\pm$ some user-defined deviation of the bounds given by the standard. Please note that this

⁶This step constitutes an approximate subset sum problem. However, no globally optimal solution is calculated here.

deviation leads to an approximate match of the desired Φ_A , but it is guaranteed to be within the bounds given by the respective standard, cf. figure 3.12. Particularly in the first iteration, when aggregates with NMA are selected, this step often overshoots the allowable pass ratio when V_D is too small. In this case the algorithm terminates and has to be restarted. Once a set of correctly sized aggregates which satisfies the pass ratio has been selected, the aggregates which have not been selected for the PSD are **retessellated**. The procedure is illustrated by taking SMA 8 S as an example. Then, $\bar{\phi}_1 = 0.05, \bar{\phi}_2 = 0.5, \bar{\phi}_3 = 0.2$, c.f. figure 3.8(a). The following equations hold (c.f. figure 3.11)

$$\Phi_{tA}\bar{\phi}_1 = \Phi_1^{\text{sel}}\varphi_1 = (1-s)^3\varphi_1 \quad (3.17)$$

$$\Phi_{tA}\bar{\phi}_2 = \Phi_2^{\text{sel}}\varphi_2 = (1-s)^6(1-\varphi_1)\varphi_2 \quad (3.18)$$

$$\Phi_{tA}\bar{\phi}_3 = \Phi_3^{\text{sel}}\varphi_3 = (1-s)^9(1-\varphi_1)(1-\varphi_2)\varphi_3 \quad (3.19)$$

$$\Phi_A = \Phi_{tA}(\bar{\phi}_1 + \bar{\phi}_2 + \bar{\phi}_3) . \quad (3.20)$$

Here, $\varphi_i = \frac{V_S}{V_{\text{sel}}}$ is the volume of aggregates with sieve size S that is required to fulfill the pass ratio over the volume of selectable aggregates. Additionally, the consistency condition holds

$$\varphi_i \leq 1 . \quad (3.21)$$

In a general form with n sieves, equation 3.20 is written as

$$\Phi_A = \sum_{i=1}^n \underbrace{\left[(1-s)^{3i} \left(\prod_{j=1}^{i-1} (1-\varphi_j) \right) \right]}_{\Phi_{tA}\bar{\phi}_i} \varphi_i . \quad (3.22)$$

This nonlinear system of equations can be solved for the $n+1$ unknowns. However, the resulting s constitutes an upper limit, since aggregates which are smaller than the sieve size threshold of 2 mm are automatically discarded after retessellation. The theoretical upper limit for a constant shrinking factor is $s = 0.0667181$. It was found that a constant value of $s = 0.05$ worked reliably. Due to the aforementioned reasons concerning gap widths, $s = \frac{i}{30}$ was used for SMA 8 S in the present study. Subsequently, the algorithm begins the next iteration with a smaller sieve size until the whole PSD is matched down to the sieve size threshold. Usually, if $\varphi_n < 1$, there are some non-selected aggregates remaining, which are now discarded, too.

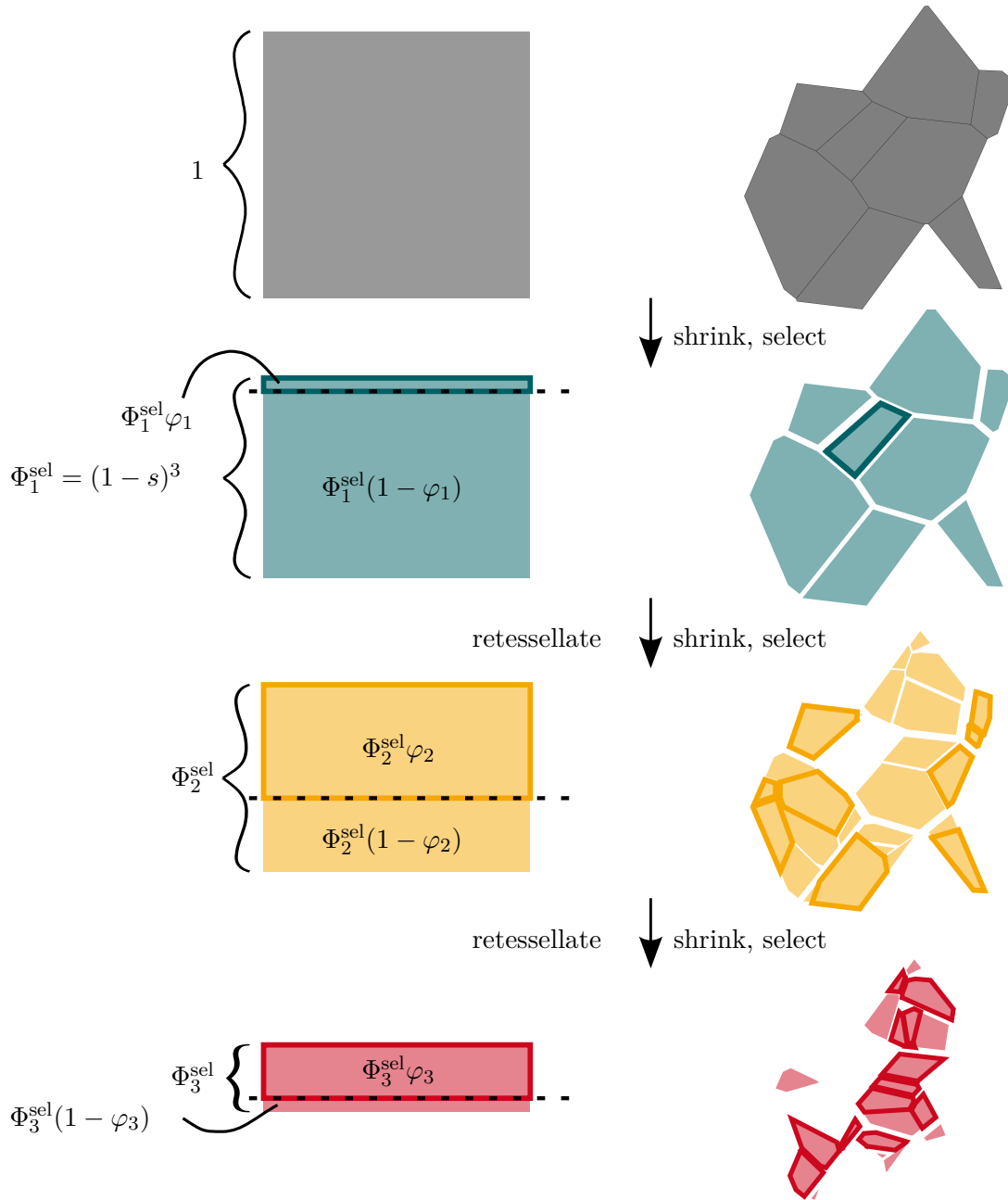


Figure 3.11: Illustration of the shrinking, selection, and retessellation steps of the nested VT algorithm.

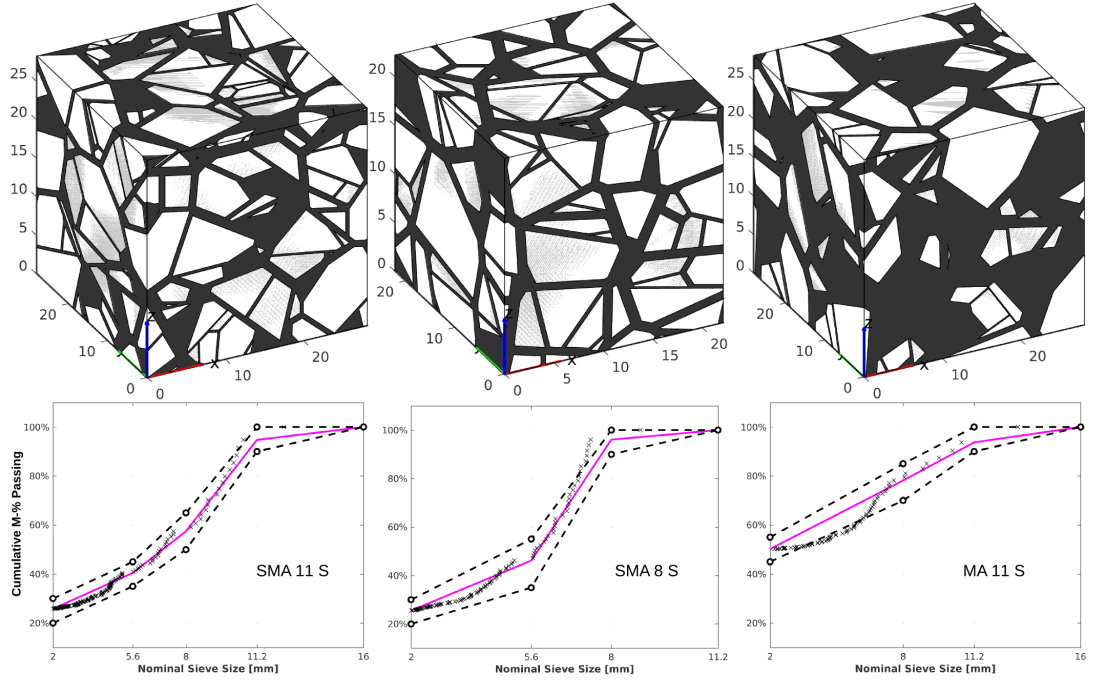
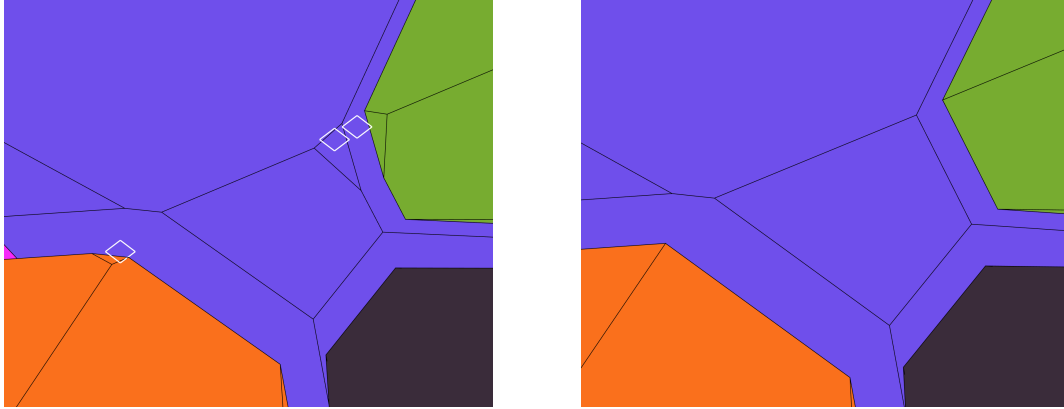


Figure 3.12: Virtual geometries of three different HMA types.

3.4.4 Geometry Regularisation

In a random VT, as it is used here, arbitrarily small geometric details occur, which lead to an unnecessary level of detail. Several remedies exist which rely on a minimal allowable distance between neighbouring seeds, weighted seeds, and centroidal VTs [56; 67; 157]. Here, the highly irregular shapes of a random VT are retained, which the authors hold to be more realistic in the case of asphalt. Typically, such a VT contains several tiny triangular facets. Naturally, the local h-refinement due to geometric details depends on the desired global mesh density. Hence, a metric based on the target characteristic element length, l_c , which will be determined in section 3.5.2, is used which removes triangular facets smaller than $\frac{\sqrt{8}}{25} l_c^2$. A new unique intersection of the three adjacent facets of the discarded triangle is computed and the facet and vertex descriptions of the affected polyhedron are updated, see figure 3.13. Using the later defined target value of $l_c = 0.5 \text{ mm}$, leads to ≈ 45 removed facets within $V_D = 12 \text{ cm}^3$. If one attempts to remove larger triangles, the intersection can lie within a neighbouring aggregate, leading to intersecting polyhedra. Therefore, some care is required to determine a sensible value.



(a) Tiny triangles provide unnecessary richness of detail. The diamond markers indicate the positions of the new intersection vertices.

(b) The regularised polyhedra.

Figure 3.13: An example of geometry regularisation. Tiny triangular facets, present in a), are removed in b).

3.5 Finite Element Based Modelling

Computational homogenisation from viscoelastic RVEs is an expensive procedure that involves the numerical solution of initial boundary value problems. In the present study, the Degrees of Freedom (DOFs) are in the order of 10^6 . Thus, several measures are taken in order to keep the numerical effort to a minimum. Concerning the solution procedure, this involves the boundary conditions, the cycles needed to achieve a steady-state solution and the timestepping. Concerning the DOF, the VT has already been modified in section 3.4.4 to reduce disadvantageous geometric properties. Furthermore, the mesh is coarsened within the aggregates, where high spatial resolution is not required.

3.5.1 Boundary Conditions and Homogenisation

The use of periodic displacement-based boundary conditions is a well established technique to obtain minimal RVEs, particularly in the context of first-order strain driven homogenisation presently used, c.f. [124; 96; 135; 152]. Here, a `python` implementation of the method described in Stier et al. [161] and applied in Bednarczyk et al. [39] is used. The displacement field $\mathbf{u}$ is decomposed into a constant far-field and a zero-mean fluctuation part

$$\mathbf{u} = \bar{\mathbf{u}} + \tilde{\mathbf{u}} = \bar{\boldsymbol{\epsilon}}\mathbf{x} + \tilde{\mathbf{u}}, \forall \mathbf{x} \in \Gamma, \quad (3.23)$$

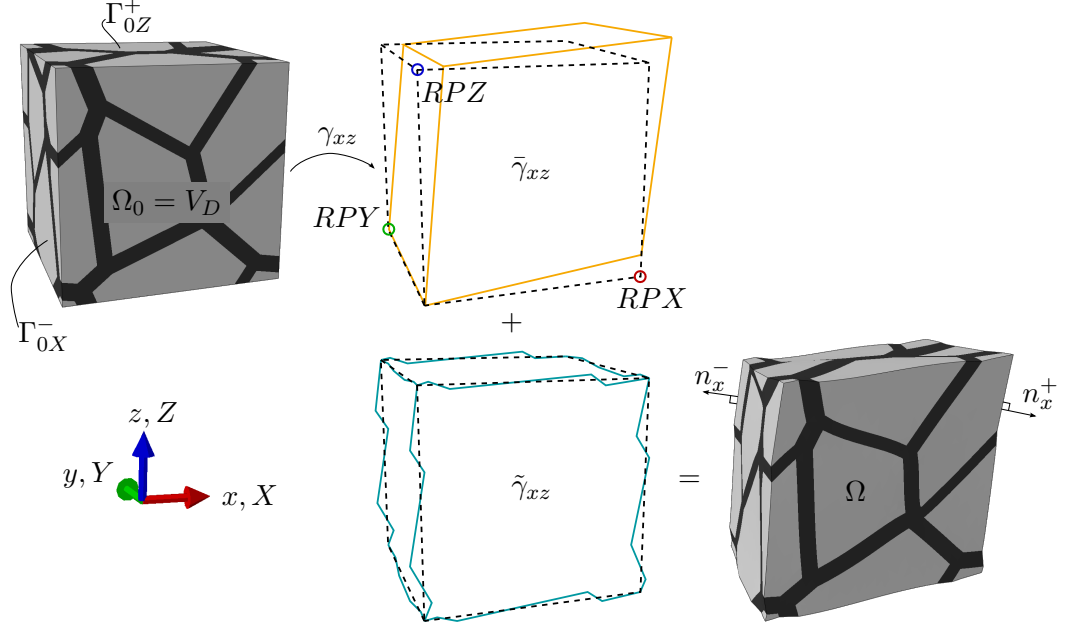


Figure 3.14: Illustration of the application of PBCs and the used nomenclature.

such that the following equations hold

$$\left. \begin{aligned} \mathbf{u}^+ &= \mathbf{u}^- \\ \mathbf{t}^+ &= -\mathbf{t}^- \\ \mathbf{n}^+ &= -\mathbf{n}^- \end{aligned} \right\} \forall \mathbf{x}^+ \in \Gamma^+ \text{ and } \mathbf{x}^- \in \Gamma^- . \quad (3.24)$$

Please see figure 3.14 for an illustration. $\mathbf{t}$ denotes the traction vector in current configuration. Superscripts $+$ and $-$ indicate faces whose normals in the reference configuration point into positive and negative coordinate directions, respectively. The complete far-field strain is described through the displacements of three reference points, $RP\{X, Y, Z\}$. Unlike in a previous publication [178], the elasticity tensor $\mathbb{C}$ is not fully populated by applying three uniaxial strain and three pure shear modes and computing the volume integrals of stress and strain. Here, only the shear response is of interest, c.f. equation 3.2. Scaled to unity, the displacement amplitudes at the reference points read

$$\gamma_{xy} : \begin{cases} u_y^{RPX} = 1 \\ u_x^{RPY} = 1 \\ u_x^{RPZ} = 0 \\ u_y^{RPZ} = 0 \end{cases} , \quad \gamma_{xz} : \begin{cases} u_z^{RPX} = 1 \\ u_x^{RPZ} = 1 \\ u_x^{RPY} = 0 \\ u_z^{RPY} = 0 \end{cases} , \quad \text{and } \gamma_{yz} : \begin{cases} u_z^{RPY} = 1 \\ u_y^{RPZ} = 1 \\ u_y^{RPX} = 0 \\ u_z^{RPX} = 0 \end{cases} . \quad (3.25)$$

For small deformations, the following approximation is valid

$$\langle \boldsymbol{\sigma} \rangle \approx \langle \mathbf{P} \rangle = \frac{1}{\Omega_0} \int_{\Gamma_0} \mathbf{T} \otimes \mathbf{X} d\Gamma_0, \quad (3.26)$$

with $\mathbf{T} = \frac{d\mathbf{f}}{dA}$ being the traction vector in reference configuration and $\mathbf{P}$ the first Piola stress. This means, that it is possible to sample the volume averaged Cauchy stress $\langle \boldsymbol{\sigma} \rangle$ from the reaction forces at the reference points and divide this value by the undeformed face area of V_D . Due to the viscoelastic material behaviour, the system requires a few cycles to reach a steady-state⁷, characterised by $d\tau_0/dt = 0$. Throughout this work, a frequency of 1 Hz is used. It was found that two full cycles are required until the shear stress amplitude τ_0 remains stable for this loading frequency, see figure 3.15. In order to reduce the computational time, the two equilibrating cycles are computed with a coarse timestepping. Then, a quarter cycle with a fine time discretisation follows that ensures a precise sampling of the stress amplitude and loss angle.

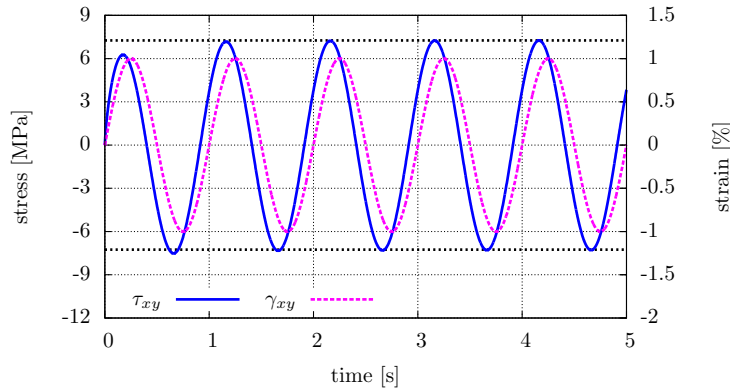


Figure 3.15: Five displacement controlled cycles of pure shear. A far-field strain amplitude of $\gamma_{xy} = 0.01$ is applied at 1 Hz. The black dotted lines indicate the steady-state stress amplitude. Two cycles are required for the stress to equilibrate.

3.5.2 Meshing

The open-source mesh generator **GMSH** [76] is used to create unstructured tetrahedral meshes. Quadratic shape functions were found to be advantageous. Strains and stresses strongly localise in the mortar and at the interface due to the material contrast. Thus, a fine discretisation is required there, but not within the aggregates.

⁷Since the transient response is not of interest, a steady-state dynamics approach in frequency domain could have been used.

Since the aggregates make up the majority of V_D , further significant savings in DOF are expected without influencing the mechanical response when the mesh is coarsening within aggregates, which is coined Intra-Aggregate Element Growth (IAEG) in the present contribution. This can allow faster computations, or make it possible to compute larger V_D s. First, mesh convergence is investigated.

Mesh Convergence

Mesh convergence is investigated for two samples of SMA 8 S of different dimensions. Since the mortar stiffness depends on the loading frequency, and the material contrast is known to influence the required mesh density, it is important to use the correct frequency here, too. Loading the mortar at 1 Hz yields a complex shear modulus of 52.34 MPa. Thus the *apparent* material contrast between aggregate and mortar, c_{AM} calculates to

$$c_{AM}(f = 1 \text{ Hz}) = \frac{G_{agg}}{G_{mortar}(f = 1 \text{ Hz})} \approx 637 . \quad (3.27)$$

Please note that this contrast only holds for a homogeneous volume of aggregate compared to a homogeneous volume of mortar under identical boundary conditions. In a composite, the strains localise in the softer phase, resulting in a higher effective loading frequency which depends on the volume fraction, geometry, and topology. Thus, the effective material contrast is a field quantity and typically lower than the apparent one.

Here, neither regularisation, nor IAEG are employed. Two different V_D are used: 10 cm^3 , and 12 cm^3 . As the number of DOF increases, a reduction in G^* and an increase in δ is observed, see figure 3.16. Albeit being small, the slope between the finest discretisations is not yet zero. However, asymptotic behaviour of G^* and δ with increasing DOF can be inferred. To make a compromise between accuracy and complexity, it is decided to use a characteristic element length, l_c , of 0.5 mm, which corresponds to ≈ 2 million DOF for the shown domain volumes.

Static Mesh Size Adaptation

Here, we use a heterogeneous mesh density in order to reduce the DOF. Unfortunately, this breaks mesh periodicity which was previously automatically satisfied using GMSH. Hence, periodicity constraints are computed and encoded in the input-file. GMSH allows to modify the local mesh density using so-called attractor nodes. Here, they are used to increase the mesh size in a sphere of influence around the nodes which are placed at the centroid of each aggregate large enough to be worth the effort. All aggregates in a domain are put into size categories using the sieve size metric from equation 3.10 and different spheres of influence are used based on these categories. Please refer to

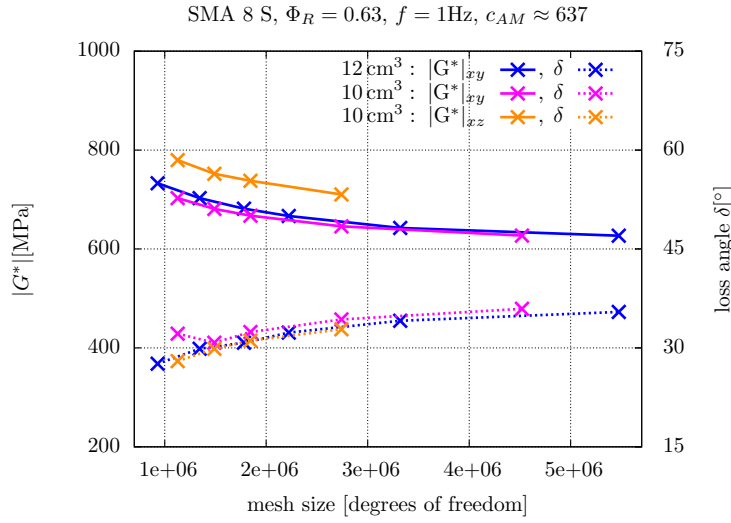


Figure 3.16: Evolution of the dynamic modulus, $|G^*|$, and the loss angle, δ , with an increasing number of DOF. For 12 cm^3 , only the modulus in xy-direction is shown. The moduli in xy- and in xz-direction are given for 10 cm^3 .

figure 3.17 for a cutaway view of a volume element exposing the heterogeneous mesh size. In its current form, typically 10 – 15% of DOF are saved. However, care must be taken not to affect the mechanical response negatively.

Mesh Optimisation

GMSH features an inbuilt mesh optimisation routine and also uses Netgen [155]. Both are employed to improve the quality of the tetrahedral mesh. In order to assess the impact of geometry regularisation, IAEG, and mesh optimisation, three samples have been tested with different combinations of these techniques, see table 3.4. The geometries are identical except for the regularisation. The mean values of DOF, the total Central Processing Unit (CPU) time, and $|G^*|$ are given. It can be seen, that the total CPU time and the number of DOF decrease when regularisation is used together with IAEG. When mesh optimisation is employed in addition, the number of DOF increases, but the total CPU time becomes even smaller. This is attributed to the larger step sizes. It can be concluded, that the aforementioned measures have a tremendous effect on the runtime of the FE simulations. The smaller system of equations and the improved element quality lead to a speedup of a factor ≈ 3 . Naturally, it has to be established that these measures do not affect the mechanical response in a negative way. The combined impact of regularisation and IAEG is negligible. Mesh optimisation reduces the stiffness mildly. However, mesh convergence (c.f. figure 3.16) has been investigated

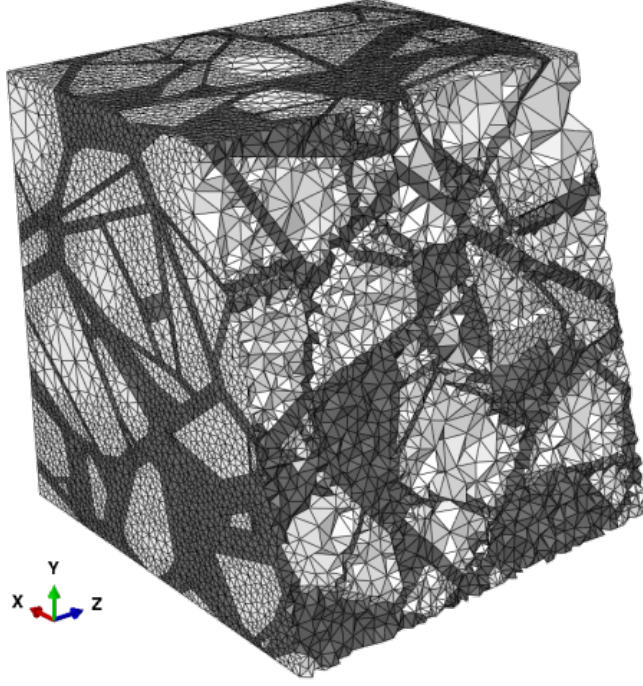


Figure 3.17: View of a virtual SMA 8 S sample with mesh coarsening within aggregates. Here, the number of DOF is reduced by 13.65% over the homogeneous mesh density.

without these techniques and a not fully converged mesh density was chosen. Hence, it is hypothesised, that the stiffness reduction due to mesh optimisation is a step in the right direction.

3.6 Results & Discussion

All following computations used regularisation, IAEG, and mesh optimisation. The scatter in the mechanical properties is captured through the standard deviation, sd , of $|G^*|$, and δ with increasing domain volume V_D . Ten different realisations are used for each V_D which is chosen in steps of 8, 12, and 16 cm³. Each sample is sheared in three modes (c.f. section 3.5.1), subsequently $|G^*|$ and δ are calculated from the data. Please note, that sd is a measure of the scatter within one sample (the anisotropy), as well as a measure of the scatter between different samples. The RVE is defined as the smallest V_D , for which the scatter reduces below a required threshold. For a single sample, this would require huge dimensions. Hence, the concept of ergodicity is employed, which states that the average result of few large samples equals the average

	DOF	CPU time [s]	$ G^* $ [MPa]
PVT	2655441	685213	718.5
reg + IAEG	2265771 (-14.67%)	310547.3(-54.7%)	718.2 (-0.04%)
reg + IAEG + opti	2456634 (-7.49%)	221958 (-67.6%)	701.9 (-2.31%)

Table 3.4: Quantification of the impact of geometry and mesh modifications. Mean values for three different sample geometries. All computations have been executed using all 16 cores of a dual CPU Xeon system running at 2.6 GHz.

result of many smaller samples, as long as the mean is not biased. For example, Kanit et al. [96] make extensive use of this concept.

3.6.1 Effective Properties of SMA 8 S

The results of the homogenisation procedure are depicted in figure 3.18. In general, the change of the properties with increasing sample size is rather weak, both $|G^*|$ and δ exhibit only negligible changes with increasing V_D . This is attributed to the fact that all samples are already representative in the sense that the PSD and Φ_A are accurately captured. Hence, it is judged that the samples are ergodic. Increasing heterogeneity would be observed if smaller volumes were cut out from these geometrically and volumetrically representative samples, which is not possible using the proposed method since periodicity would be lost. The coefficient of variation is rather stable at values slightly below 10%, which is close to the values reported by Romero and Masad [149] for a mixture with 12.5 mm NMA under three different test scenarios. Interestingly this is a value that was also determined to be asymptotic by Kim et al. [101] for two dense graded asphalt types based on geometrical considerations. Since the geometry generator terminated more reliably for $V_D = 12 \text{ cm}^3$ and it is more likely that this V_D is geometrically representative in reality, it was decided to sample the effective properties from this volume.

	$ G^* $ [MPa]	δ [°]
SMA 8 S	738.18 ± 49.37	30.8 ± 0.93
PVT 9.2 mm	591.87 ± 67.36	37.26 ± 1.17
PVT 4.8 mm	721.47 ± 31.53	28.47 ± 0.62

Table 3.5: Effective properties of SMA 8 S and apparent properties of PVTs with 9.2 mm and 4.8 mm mean sieve size. All domain volumes measure 12 cm^3 and 10 realisations have been used for each geometry type. Mean values and standard deviations are given.

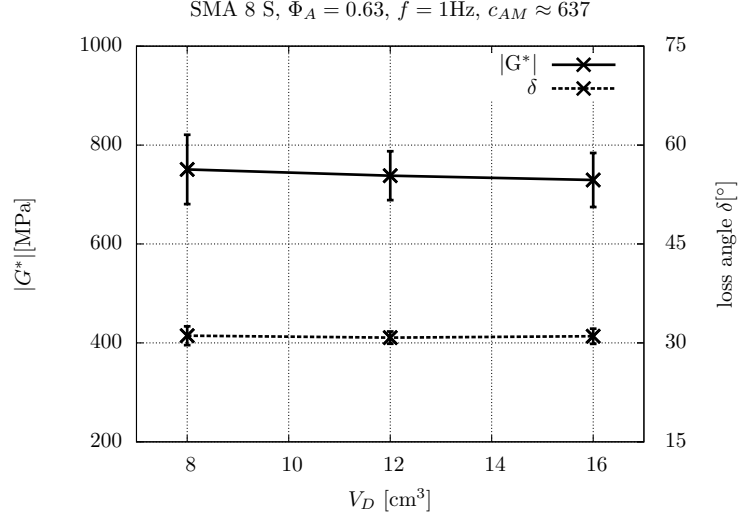


Figure 3.18: Evolution of the average of $|G^*|$ and δ with increasing V_D . The errorbars show the standard deviation.

3.6.2 Influence of the Particle Size Distribution

In order to highlight the importance of capturing the PSD accurately, simulations of a PVT of $V_D = 12\text{ cm}^3$ with 9.2 mm and 4.8 mm mean sieve sizes have also been run. Since the same V_D has been used and no study of representativeness is conducted for the PVT volume elements, their properties must not be called representative, but apparent instead. The properties of SMA 8 S, and both PVTs are given in table 3.5. It can be seen that using a polydisperse particle distribution increases the stiffness and lowers the dissipation with respect to the PVT with 9.2 mm mean sieve size. Decreasing the mean sieve size to 4.8 mm increases the stiffness again and leads to properties which are approximate to those of SMA 8 S. These differences are attributed to the localisation of strains and stresses in mono- and polydisperse particle distributions. figure 3.19 shows the distributions of von Mises stress for all sample types. The differences are further highlighted by histograms of stress and strain of one showcase realisation of each geometry type, see figure 3.20 and figure 3.21. The coloured filled curves show the relative local volume, i.e. the volume governed by stress/strain level over V_D . The black lines provide the cumulative volume over stress/strain, i.e. the integral of the filled curves. The difference in the asymptote of cumulative volume is attributed to the fact that the SMA 8 S sample does not feature the target aggregate volume fraction Φ_A exactly, as mentioned in section 3.4.3. Although the difference is small, this can be a potential bias. However, this is ruled out for the monodisperse

PVTs samples with different mean sieve sizes for which the respective Φ_{AS} match exactly.

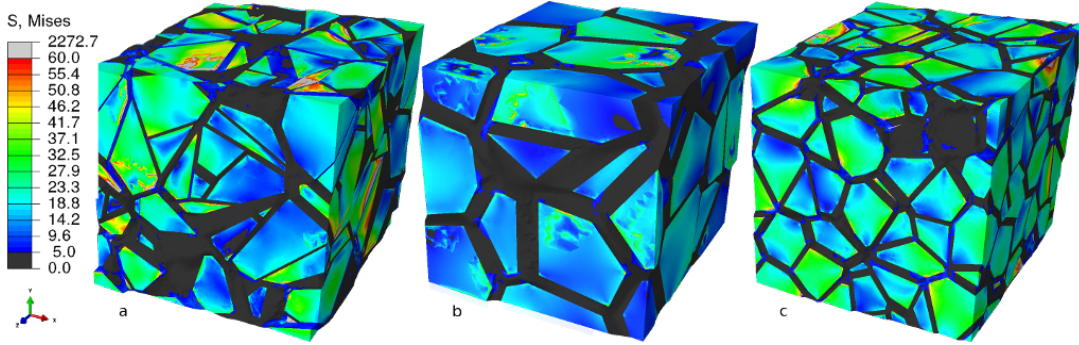


Figure 3.19: Von Mises stress field within the aggregates of a sample of SMA 8 S (a), a PVT with 9.2 mm mean sieve size (b) and a PVT with 4.8 mm mean sieve size (c). The stresses are truncated at 5 and 60 MPa. A far-field strain of $\gamma_{xy} = 0.01$ is applied. The deformation is exaggerated by a factor of 10. The complex shear moduli, $|G_{xy}^*|$, of the samples are 711 MPa (a), 573 MPa (b), and 761 MPa (c).

The histograms show, that the stresses and strains in the mortar phase differ weakly. The histograms largely overlap and the cumulative curves almost coincide, see Figures 19 & 20 (a). It is judged that the stress and strain localisations within the mortar cannot explain the strong difference in the homogenised properties, cf. table 3.5. However, a significant difference can be inferred from the histograms of stress and strain in the aggregate phase, see (b) in both figure 3.20 and figure 3.21. There, it is shown that the distributions are significantly shifted to higher levels and that the bandwidth is increased. Due to the elastic nature of the aggregates, stress and strain histograms exhibit high similarity. These shifts are attributed to the larger surface area of the aggregates in the 4.8 mm monodisperse and the polydisperse samples than in the 9.2 mm monodisperse sample types. The larger total surface area enables improved transfer of stress and strain between mortar and aggregate phase. This can be seen as an example of Galilei's "square-cube law" which states that the volume of a body decreases with linear dimension (here: sieve size) to the power of three, but the area only with power of two, leading to higher surface to volume ratios for small sized aggregates.

3.6.3 Loading Frequency Dependence of the Response

In a previous study using PVTs and linear elastic material for both phases [178], it was found that RVE size increased with increasing material contrast. This result can be transferred to linear viscoelastic modelling, where the scatter increases reciprocally to

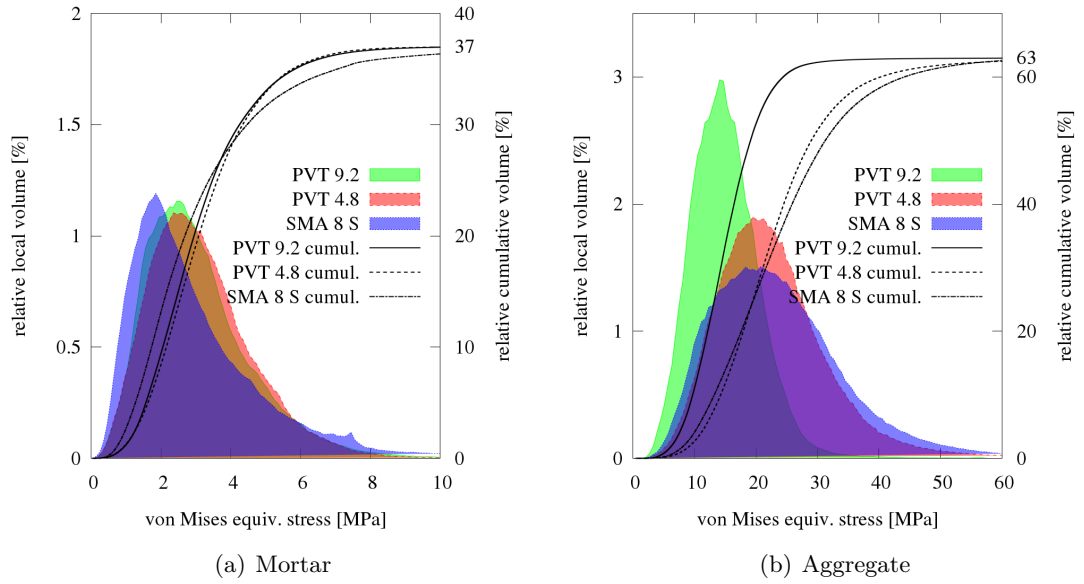


Figure 3.20: Stress histograms of the von Mises equivalent stresses. In (a), the stress distributions in the mortar are given for all three sample types. The differences are not significant and would probably look qualitatively different for a different set of realisations. In (b) however, it can be seen that changing the geometry from large to smaller or polydisperse aggregates significantly alters the distribution to higher stress levels.

loading frequency. figure 3.22 shows the results of a set of five realisations of a 9.2 mm PVT. The sets share identical geometry, just the loading frequency has been changed to 0.01 Hz and 100 Hz. The errorbars clearly indicate an increasing scatter for lower frequencies. This finding has also been reported for the linear viscoelastic regime by Ozer et al. [141] using a plane strain model and by Zhang and Ostoja-Starzewski [188] for plane stress state. Please note that the response for 1 Hz is stiffer than given in table 3.5 since a coarser mesh has been used here.

3.7 Conclusions & Outlook

The numerical homogenisation shows that the effective response can be obtained once geometrical representativeness is given. $V_D = 12 \text{ cm}^3$ suffices to predict the response with an accuracy that was also found to be asymptotic through real experiments. Then, the scatter hardly decreases with increasing sample size. This holds at least for the investigated frequency of 1 Hz and the resulting material contrast, meaning that

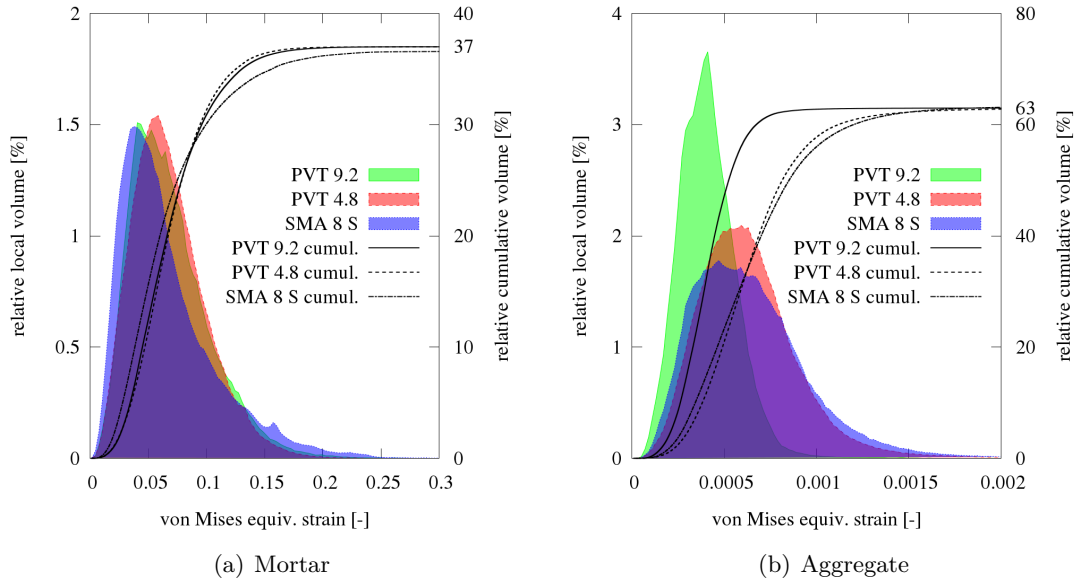


Figure 3.21: Strain histograms of the von Mises equivalent strains. In (a), the strain distributions in the mortar are given for all three sample types. Again, the differences are hardly discernible. It can be inferred from (b), that the distribution seen in figure 3.20 is also present in strain space, which is due to the elastic behaviour of the aggregates. The distribution is stretched to higher strain levels for smaller and polydisperse aggregate sizes.

higher frequencies can be applied safely, but care should be taken for lower frequencies. Please note that a complete set of dynamic moduli to characterise (asymptotically) isotropic solids has not been established through homogenisation, here. However, this is easily achieved by applying different far-field strains.

The relatively high Φ_A in the HMA type investigated here raises the question whether constitutive modelling in the small-strain regime is justified, albeit small far-field straining. Due to the localisation, strains in the mortar are amplified over the far-field strain. Schüller et al. [157] investigated the need to perform finite-strain modelling for the mortar, but found that its impact is negligible, at least without damage modelling. Although areas of large strain exist, their volume is too small to have a significant impact on the bulk response.

Clearly, the computational efficiency of geometry and mesh can be improved. Only mild geometry regularisation was used in the present study. More advanced concepts could use the normal distance of the intersection point from the discarded triangle, search for intersecting polyhedra, and remove triangles based on metrics which take

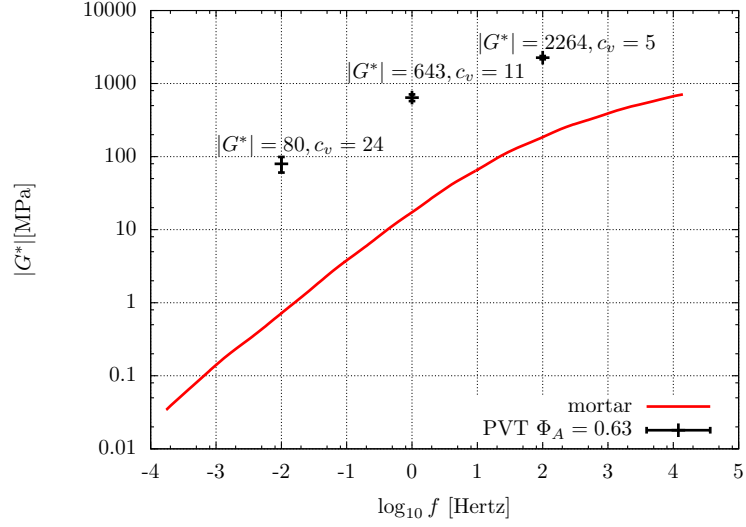


Figure 3.22: Evolution of the average of $|G^*|$ with changing frequency. The errorbars show the standard deviation. The mortar properties are given for comparison. The results deviate from those given in table 3.5 since a coarser mesh has been used.

aspect ratios into account, etc. Naturally, a repulsion distance between neighbouring aggregates could be introduced as well. All these concepts should be critically evaluated based on comparison between real and virtual geometry and topology. Also, IAEG can be more aggressive. An improved method could be the generation of a shrunk twin within each aggregate, which contains only larger elements.

As mentioned in section 3.4.2, the bitumen in the mortar is overdosed due to the negligence of adsorbed binder. As a result, mortar and composite stiffness are probably underestimated. Karki et al. [98] have tested mortar specimens in a similar setup to the one described here and determined a stiffer response. Please note, that their mortar mixtures differ from those used here, though. However, a stiffer mortar would not change the qualitative results, since the lower c_{AM} from a stiffer mortar constitutes an even better scenario for computational homogenisation.

Furthermore, the geometrical and topological properties of the virtual specimens require more attention than just capturing the PSD. The realism of the current aggregate geometries requires additional research. Shape, angularity, and orientation are only some factors that can be computed from real and virtual samples. How VTs can be finetuned to mimic other geometric properties is an open question. In metallurgy for example, using Voronoi tessellations for virtual grain structures is an active research area, see e.g. Zhang et al. [189]. Sophisticated software for virtual geometry genera-

tion exists, such as **Neper** [145]. Since most properties of the resulting aggregates are determined by the seed lattice, one could think of an anisotropic seed density. However, this would simultaneously alter orientation and shape distributions. Particular attention should be attributed to the surface area of the aggregates, since the amount of adsorbed binder depends on it. Unfortunately, this is a quantity that is difficult to measure [58]. It might be possible to determine correction factors for the errors made through representing rough, and not necessarily convex aggregates found in reality by smooth Voronoi polyhedra.

The versatility of the developed framework allows to model a whole family of HMA mixtures. However, the accuracy of representation has yet to be determined. The authors aspire to validate the present approach in upcoming works.

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4 Digital sieving of irregular 3D particles — a study using XRCT and statistically similar synthetic data

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J. Neumann wrote the particle analysis code in `Matlab`, acquired synthetic data, analysed the results, and wrote the article.

J.-W. Simon and S. Reese provided intellectual content and gave conceptual advice.

All authors drafted the work for intellectual content.

S. Reese was engaged in obtaining funds for the research.

All authors proofread and edited the manuscript.

All authors approved the publication of the final manuscript.

4.1 Abstract

The properties of particulate materials are influenced by purely geometric properties like size, size distribution, and shape. However, size is an ambiguous quantity for non-spherical particles. Therefore, the impact of particle shape on the size as measured by several common and original estimators is investigated. Particularly, a high-fidelity digital sieving method based on the first principal axis of a particle is proposed. An XRCT scan of asphalt concrete is analysed for the shape distribution and its compliance with typical standards. Then, a larger synthetic particle set with a statistically similar, but slightly more extreme shape distribution is generated for testing the size estimators. It is found that the equivalent volume sphere should be abandoned and alternatives are proposed. The analysis is based on simple discrete computational geometry and can easily be implemented.

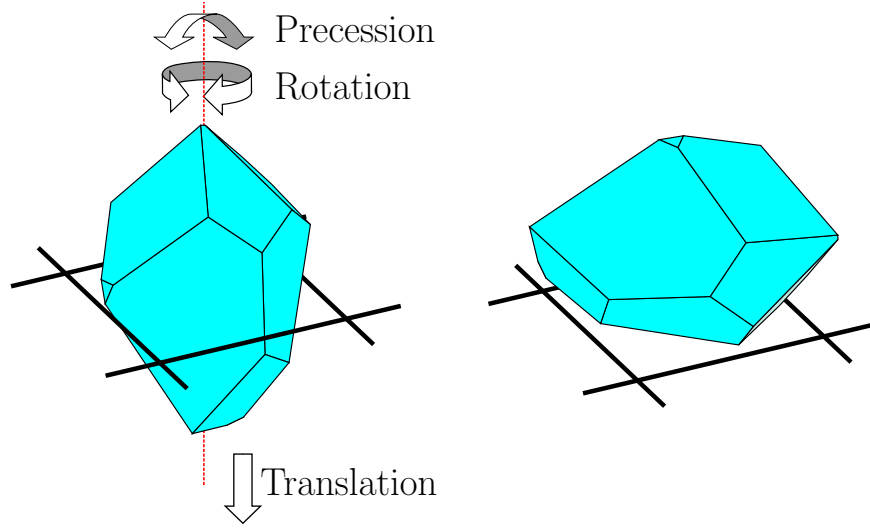


Figure 4.1: Illustration of a convex polyhedron passing through its sieve along its major axis. The minimum sieve size is found by rotating the particle around its major axis. Other orientations are assumed to yield larger sieve sizes.

4.2 Introduction

Numerical simulations of particulate materials are either based on image, or on synthetic data of particle geometries. Synthetic data is attractive since its generation is fast and cheap. However, the realism of the aggregate shapes is critical, as Yang et al. [183] emphasised in a review article about heterogeneous modelling efforts of stone based materials. The properties of particulate composites in general, and of asphalt in particular, depend on purely geometric properties like size, size distribution, shape, surface area and orientation of reinforcing particles [40; 170; 171; 41]. Particle size is usually analysed via image analysis, or by sieving, cf. [28]. Sieve analysis is probably one of the oldest methods to categorise particles by size. It is still in widespread use, particularly in road engineering, where it is required that the PSD is established via sieving [8; 12]. The S of an aggregate particle is defined as the edge length of the smallest *quadratic* aperture, through which the particle can pass in at least one direction, cf. figure 4.1. However, sieving has the disadvantage that it produces only piece-wise lower bounds of S . Furthermore, the actual simulation of the process would be challenging, e.g. a discrete particle simulation with an abundance of contact pairs. Thus, it is worthwhile to establish the individual sieve size without actually simulating the process of sieving.

Next to size, particle shape plays an equally important role. Standardised measures in road engineering include the flat and elongated ratio (also called flakiness), which

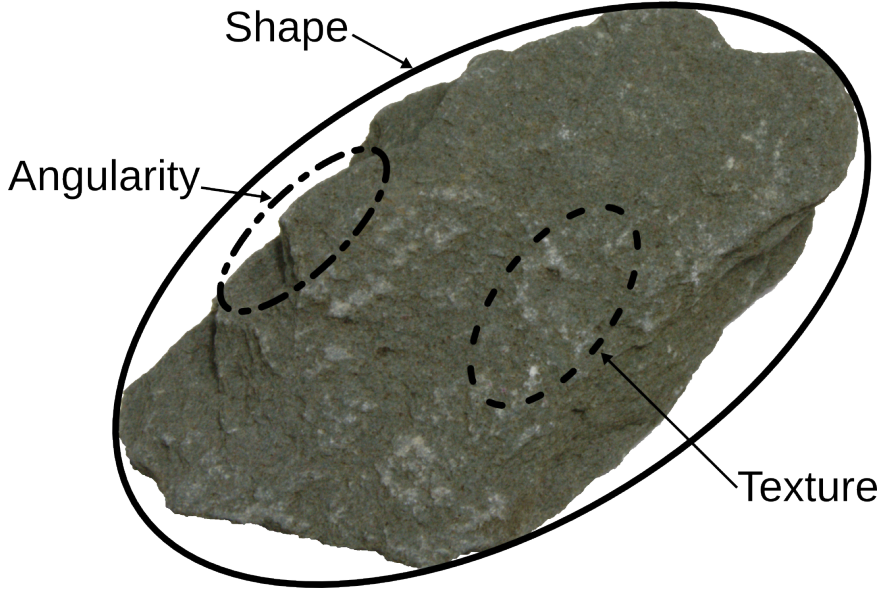


Figure 4.2: Illustration of the different scales on which shape, angularity and texture are defined.

is established by bar sieving [9], and the shape index [4; 19], which requires measurement with a sphericity vernier calliper. In the present work, the differentiation of descriptors for irregular particles into shape, angularity and texture quantities by Tutumluer et al. [170] is adopted, cf. figure 4.2. Please note that angularity and surface texture are not a subject of the present investigation. However, the discrete particle geometries used here are fully angular, thus corresponding to angularity class $C_{100/0}$ [64]. Ratios of linear particle dimensions are often used as shape descriptors. Here, they are based on the principal axes of inertia, cf. section 4.3.1. Afterwards, several sieve size estimators are introduced in section 4.3.2. Particularly, a high-fidelity sieve size estimator is proposed which assumes that the minimal sieve size of a particle is found orthogonal to its major axis, cf. figure 4.1. The shape index is introduced in section 4.3.3. A supplementary and more sophisticated quantity is the sphericity, introduced in section 4.3.4 alongside Zingg's shape classification diagram [193; 103]. In the present work, sphericity plays a pivotal role, because the accuracy of several size estimators is assessed as a function of sphericity.

Up to the recent years, micromechanical modelling of asphalt concrete was mostly executed in 2D. However, the usage of 2D models has been shown to be problematic. Fakhari Tehrani et al. [59] reasoned that 2D approaches are only valid in the case of low aggregate volume fractions and high loading frequencies. Furthermore, several

research groups concluded that a 2D model underestimates the stresses w.r.t. a 3D model [127; 47; 46; 141].

Similar constraints did exist for the size and shape analysis of aggregates. The research group of Mora and Kwan estimated 3D properties like sphericity, flakiness, and convexity from 2D projections by assuming self-similarity of aggregates from the same source [129; 106; 130]. The same approach was used by Maerz [118] using a conveyor belt setup. A well-known rotating tray system has been developed by the US Federal Highway Administration [74], please see e.g. [27; 41; 176] for applications. However, 2D methods of sieve size analysis from image data implicitly assume that the major particle axes are always normal to the image plane [82; 107; 83].

Noteworthy intermediate steps between 2D, and full 3D measurements have been proposed by Kuo et al. [104] and Fernlund's group [63; 164], who took two images of the entire aggregate sample, in lying and in standing position. Hence it was possible to identify the shortest and longest dimensions since the intermediate dimensions were measured in both images. The same approach has been used by Chen et al. [45]. Tutumluer et al. [170] took pictures of particles from three orthogonal directions using a conveyor belt setup.

Nowadays, 3D micromechanical investigations and numerical homogenisation approaches of AC gain popularity, due to increasing availability of the imaging systems, dropping costs, and increased computational resources. Image based and synthetic approaches exist. 3D imaging methods include XRCT [70; 114; 176; 71] and 3D laser scanning [109; 72; 110; 31]. Asahina and Taylor [33] compared measurements from 3D laser scanning to XRCT and found good agreement for surface and volume between both methods.

3D image based simulation models of asphalt concrete typically rely on XRCT scanned samples [105; 47; 184; 157; 115], whereas synthetic approaches can be found in the works of Chen et al. [46]; Schüller et al. [157], and Neumann et al. [132], for example. Image based approaches guarantee geometric realism if the scanned samples are large enough, have been properly produced and image postprocessing was performed in a sensible manner. The synthetic approaches, however, need to find an estimator for the individual sieve size of particles in order to match the size distribution and care about shape properties. Recent works in this direction used extruded polygons [46] or VP [157; 132]. For reasons of simplicity, most groups estimated particle size using the diameter of the equivalent volume sphere, Equivalent Volume Sphere (EVS) [157; 132]. Alternatively, Chen et al. [46] used the width, i.e. the length of the minor axis of their extruded polygons.

In order to investigate the impact of particle shape on estimated size, the present work proceeds as follows. Size and shape data of XRCT-scanned aggregates for use in road construction are presented in section 4.3.5. Since it is questionable, whether this set is large enough, a larger, statistically similar, but more extreme synthetic particle data set is analysed in section 4.3.6. Subsequently, the uniqueness of the linear particle

dimensions is critically assessed in section 4.5.1. Results of the sieve size estimators for the synthetic particle data are shown in section 4.5.2. Finally, the impact of different estimators on the particle size distribution of the XRCT-scanned set are presented in section 4.5.4.

The methods described in the present paper are completely general and can be applied to any particulated geometries. The application in road engineering merely serves illustrational purposes.

4.3 Methodology

Typical morphology measures require linear, quadratic and cubic dimensions of the particle under investigation. In the present work, area measurements are avoided.

4.3.1 Volume and Linear Dimensions

In the following, the three linear dimensions are defined to be mutually orthogonal. Adopting the notation used in ASTM standard D4791 [4], the maximum dimension is the length, L , followed by width, W , and thickness, T , such that

$$L \geq W \geq T. \quad (4.1)$$

ASTM D4791 furthermore specifies that W is the maximum dimension in the plane perpendicular to the length and thickness and that T is the maximum dimension in the plane perpendicular to the length and width. These definitions make measurements error-prone, please refer to section 4.5.1 for a discussion. Thus, a different methodology is pursued here. An eigenvalue decomposition of the inertia tensor, also known as principal component analysis, is performed in order to establish the linear dimensions. This is done in a discrete fashion based on a tetrahedralisation of the aggregate domain. Please note, that it is not necessary to compute the inertia tensor using tetrahedralisation. Alternatively, spherical harmonics [70; 166; 42; 73; 163] or a structured mesh can be used. The latter means it is possible to work directly with the voxel data from XRCT scans, as performed by Lin and Miller [114] and in the section 4.4. The methodology is inspired by Zhang and Chen [186]. Any tetrahedron can be described by 4 distinct nodes in 3D space. To begin with, the coordinate vector of the centroid of tetrahedron i is defined via

$$\mathbf{r}_i = \frac{1}{4} \sum_{j=1}^4 \mathbf{x}_{ij}, \quad (4.2)$$

where $\mathbf{x}_{ij}$ is the nodal coordinate vector of node j . In the following, a homogeneous density $\rho = 1$ is assumed. Then, mass is defined as $m_i = \rho V_i = V_i$, with the tetrahedral volume being given by

$$V_i = \frac{1}{6} \begin{vmatrix} 1 & x_{i1} & y_{i1} & z_{i1} \\ 1 & x_{i2} & y_{i2} & z_{i2} \\ 1 & x_{i3} & y_{i3} & z_{i3} \\ 1 & x_{i4} & y_{i4} & z_{i4} \end{vmatrix}. \quad (4.3)$$

Please note that the volume of the particle, V , can already be established through summation of all tetrahedral volumes

$$V = \sum_{i=1}^{\#tets} V_i. \quad (4.4)$$

The first moment of mass distribution, $\mathbf{m}$, is defined by summation over all tetrahedra according to

$$\mathbf{m} = \sum_i V_i \mathbf{r}_i, \quad (4.5)$$

From equation 4.5, the particles centroid, $\mathbf{c}$, is the volume weighted mean of the nodal coordinate vectors of the centroids of its tetrahedra

$$\mathbf{c} = \frac{\sum_i V_i \mathbf{r}_i}{V}. \quad (4.6)$$

The second moment of mass distribution, $\mathbf{M}$, is defined by summation over all tetrahedra according to

$$\mathbf{M} = \sum_i m_i \mathbf{r}_i \otimes \mathbf{r}_i, \quad (4.7)$$

Hence, the inertia tensor, $\mathbf{\Theta}$, is defined as

$$\mathbf{\Theta} = \mathbf{I}(\mathbf{M} \cdot \mathbf{I}) - \mathbf{M}, \quad (4.8)$$

where $\mathbf{I}$ is the second order identity tensor. Next, $\mathbf{\Theta}$ is subjected to an eigenvalue decomposition fulfilling

$$\mathbf{\Theta} \mathbf{v}_i = \Theta_i \mathbf{v}_i, i = 1 \dots 3, \quad (4.9)$$

which yields three eigenvalues Θ_i and their corresponding eigenvectors $\mathbf{v}_i$. Please note that $\mathbf{\Theta}$ is symmetric and positive definite yielding strictly positive eigenvalues. The eigenvalues are the principal moments of inertia of the particle, and the eigenvectors are the associated principal axes. Furthermore, the matrix of eigenvectors, sorted according to decreasing magnitude of the corresponding eigenvalues

$$\mathbf{Q} = \begin{bmatrix} \mathbf{v}_L & \mathbf{v}_W & \mathbf{v}_T \end{bmatrix} \quad (4.10)$$

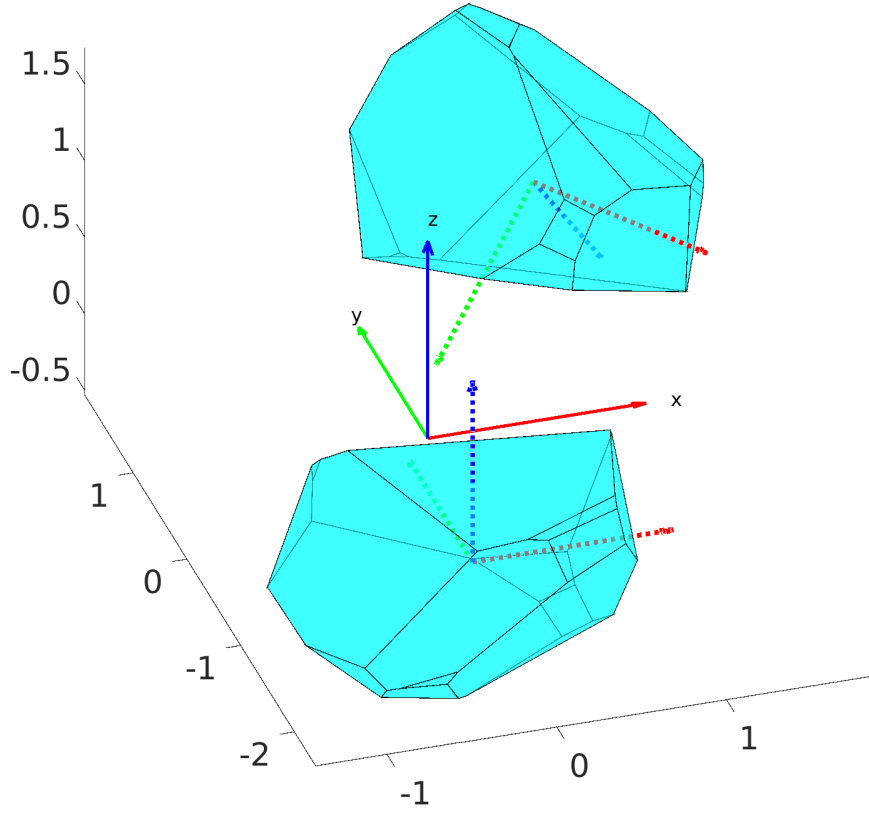


Figure 4.3: Illustration of the rotation from the particle coordinate system to the global coordinate system. A translation is included here to prevent overlap.

constitutes a rotation matrix which is used to rotate the particle from the body coordinate system to the global coordinate system, cf. figure 4.3. For some particle shapes it may happen that the eigenvectors from solving equation 4.9 are not unique, in that case $L = W = T$ and orientation in space is arbitrary (e.g. for spheres). However, this is hardly a problem in road engineering. Now, the triaxial dimensions are sampled via

$$\begin{bmatrix} L & W & T \end{bmatrix} = \max(\mathbf{x}) - \min(\mathbf{x}) , \quad (4.11)$$

where $\mathbf{x}$ is the nodal coordinate vector of the whole particle.

Mesh convergence

The accuracy of the principal component analysis depends on the discretisation. In order to establish the required mesh density several polyhedra are chosen as model problems. For regular shapes, the principal moments of inertia can be computed

analytically. Here, analytical values are computed for two bricks with dimensions $4 \times 2 \times 1$, and $5 \times 3.2 \times 0.5$ ($L \times W \times T$). In the first case, the principal moments of inertia are

$$\Theta_1 = T \int_{-\frac{L}{2}}^{\frac{L}{2}} \int_{-\frac{W}{2}}^{\frac{W}{2}} (x^2 + y^2) dx dy = \frac{8(L^2 + W^2)}{12} = \frac{40}{3}, \quad (4.12)$$

$$\Theta_2 = W \int_{-\frac{L}{2}}^{\frac{L}{2}} \int_{-\frac{T}{2}}^{\frac{T}{2}} (x^2 + z^2) dx dz = \frac{8(L^2 + T^2)}{12} = \frac{34}{3}, \text{ and } \quad (4.13)$$

$$\Theta_3 = L \int_{-\frac{W}{2}}^{\frac{W}{2}} \int_{-\frac{T}{2}}^{\frac{T}{2}} (y^2 + z^2) dx dz = \frac{8(W^2 + T^2)}{12} = \frac{10}{3}. \quad (4.14)$$

In the same fashion, the principal moments of inertia of the second brick are $\Theta_1 \approx 23.4933$, $\Theta_2 \approx 16.8333$, and $\Theta_3 = 6.9933$. Since the computation is size and shape dependent, the analysis is also conducted for a showcase VP and four XRCT-scanned polyhedra with extremal values of volume and convexity, c.f. section 4.3.5.¹ Analytical computations are not feasible for the irregularly shaped polyhedra. Thus, the relative error is measured versus a very fine discretisation. The model polyhedra are rotated around their centroids using an arbitrary rotation matrix $\mathbf{R}$. Several tetrahedralisations are generated, for which a maximum tetrahedron size, h_{max} , is chosen according to the rule

$$h_{max} = \frac{\sqrt[3]{V}}{d}, d \in 4, 6, 8, 10, 12, 15, 20, 30, 50, 75. \quad (4.15)$$

Then, Θ is computed using equation 4.8, and the principal component analysis is executed. The resulting principal moments of inertia are plotted in figure 4.4. There, it can be seen that choosing $d = 12$ allows to establish all Θ_i with higher accuracy than 99%. Hence, this value is used throughout the remaining work. We furthermore confirm that the computed principal axes are the transpose of $\mathbf{R}$, i.e.

$$|(\|\mathbf{QR}\|_2 - 1)| < 1 \times 10^{-8}. \quad (4.16)$$

4.3.2 Sieve Size Estimators

In the following, several methods to estimate the sieve size are introduced. Common to all methods presented here is the assumption that a given particle passes through its sieve along their major axis, $\mathbf{v}_L$ cf. figure 4.1. A depiction of all sieve size estimators is presented in figure 4.5. Also the colour-coding used throughout the article is shown there. The hull of the wireframe corresponds to the outline of the projected polygon.

¹The set of seven polyhedra is available for download as supplementary material.

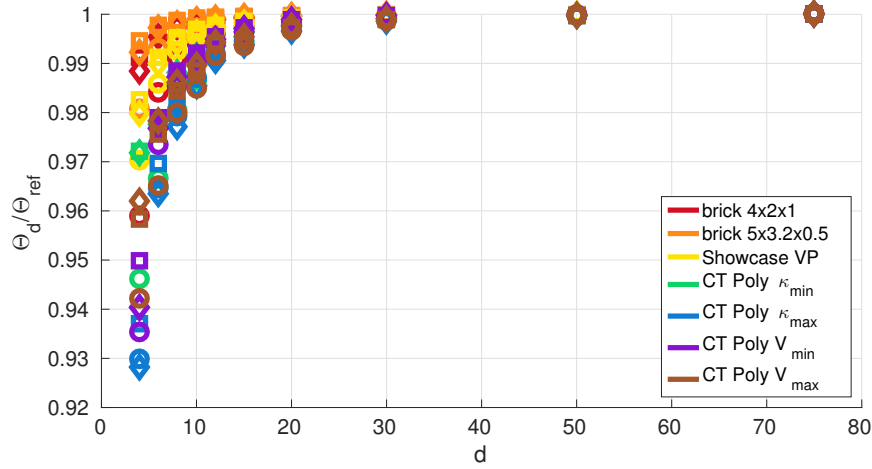


Figure 4.4: Convergence of the numerically determined principal moments of inertia to their reference solutions. Reference means analytical for the two bricks and numerical with a very fine discretisation for all other polyhedra. Using $d = 12$ leads to $\approx 1.3 \times 10^4$ tetrahedra, whereas the reference solution using $d = 75$ leads to $\approx 3.4 \times 10^6$ tetrahedra.

Equivalent volume sphere

The sieve size is often defined as the diameter of the equivalent volume sphere (EVS) [173; 157; 132]

$$S_{EVS} = \sqrt[3]{\frac{6V_p}{\pi}}, \quad (4.17)$$

where V_p is the volume of the particle. The volume can be established using e.g. Archimedes' method, analytical formulas for simple shapes, or numerical methods as in section 4.3.1.

Equivalent dimension ellipsoid

With the triaxial dimensions established from equation 4.11, the Equivalent Dimension Ellipsoid (EDE) can be established. It passes through its sieve with intermediate and minor axes aligned with the diagonals of the aperture, cf. figure 4.6. Exploiting that the aperture edges are tangential to the ellipsoid minor circumference, S_{EDE} is calculated via

$$S_{EDE} = \frac{\sqrt{2(W^2 + T^2)}}{2}. \quad (4.18)$$

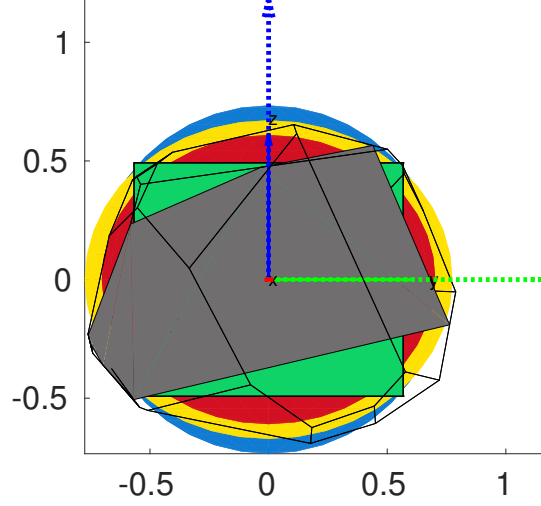


Figure 4.5: Different model shapes as viewed along L -axis. The showcase VP from figure 4.8(a) is shown as a wireframe, together with the slice of maximum S_{SLICE} . Behind it are the **EVB**, **EVE**, **EDE**, and **EVS**.

Equivalent volume ellipsoid

The equivalent volume ellipsoid, Equivalent Volume Ellipsoid (**EVE**), is an isotropically scaled version of the **EDE**, such that its volume is identical to the original particle. Its triaxial dimensions are calculated via

$$\tilde{L}\tilde{W}\tilde{T} = \frac{V_p}{V_{\text{EDE}}}LWT, \quad (4.19)$$

and identical proportions (isotropic scaling)

$$\frac{\tilde{L}}{L} = \frac{\tilde{W}}{W} = \frac{\tilde{T}}{T} = \sqrt[3]{\frac{V_p}{V_{\text{EDE}}}}. \quad (4.20)$$

Usually, $V_p < V_{\text{EDE}}$ holds. Resulting in the fact that when equation 4.18 is used to calculate

$$S_{\text{EVE}} = S_{\text{EDE}}(\tilde{W}, \tilde{T}), \quad (4.21)$$

the estimator based on the **EVE** yields a smaller sieve size than S_{EDE} . However, this is not general. E.g. for a box, S_{EVE} would be larger than S_{EDE} .

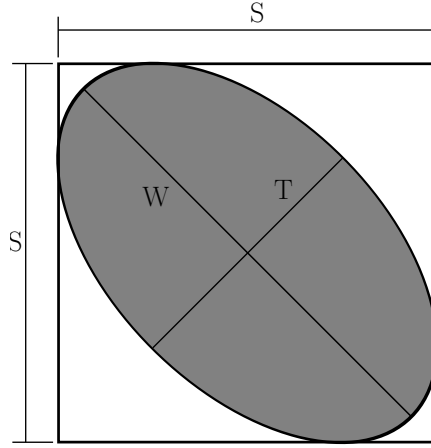


Figure 4.6: Illustration of an ellipsoid passing through its sieve.

Equivalent Volume Box

The triaxial dimensions, $\hat{L}$, $\hat{W}$, and $\hat{T}$ of the equivalent volume box, Equivalent Volume Box (EVB), are calculated in the same fashion as for the EVE using the ratio

$$\hat{D} = \sqrt[3]{\frac{V_p}{LWT}} D, \forall D \in L, W, T. \quad (4.22)$$

Depending on the width to thickness ratio, a box passes through its minimal square either with its edges aligned to that of the square, or rotated by $\pm 45^\circ$ around the major axis. Thus, there is a case differentiation for S_{EVB} , cf. figure 4.7.

$$S_{EVB} = \begin{cases} \hat{W} & \text{if } \frac{\hat{T}}{\hat{W}} \geq \sqrt{2} - 1 \\ \frac{\hat{W} + \hat{T}}{\sqrt{2}} & \text{if } \frac{\hat{T}}{\hat{W}} < \sqrt{2} - 1 \end{cases}. \quad (4.23)$$

Slice orthogonal to major axis

In order to assess the accuracy of the different abstract shapes in predicting S , a highly precise method is used. Therefore, the intersections of the edges of the particle with planes orthogonal to v_L are computed, please see figure 4.8(a) for a depiction using four slices.

The resulting polygons are subsequently rotated around $\mathbf{v}_L$ in steps of 1° . The minimum of the maximum of y- and z-dimensions is then taken to be S_{SLICE} . Please note that the configuration for the minimal aperture is generally not a one that has one of the edges of the polygon aligned with y-, or z-dimension. This is in contrast to the

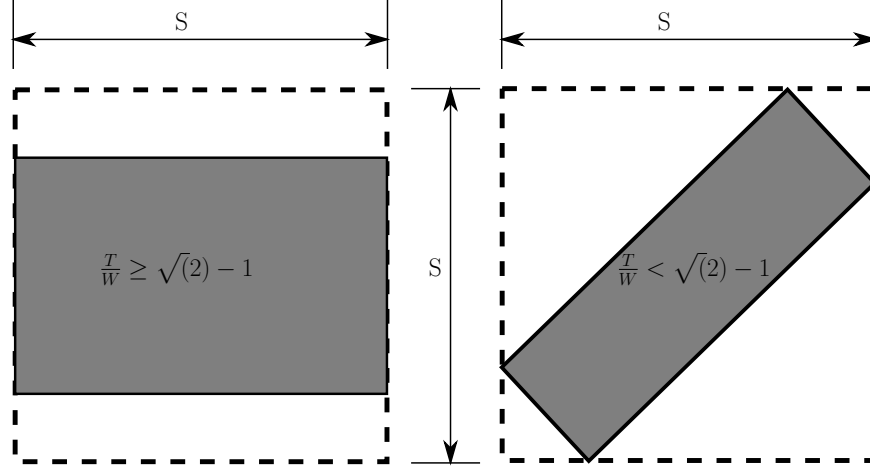


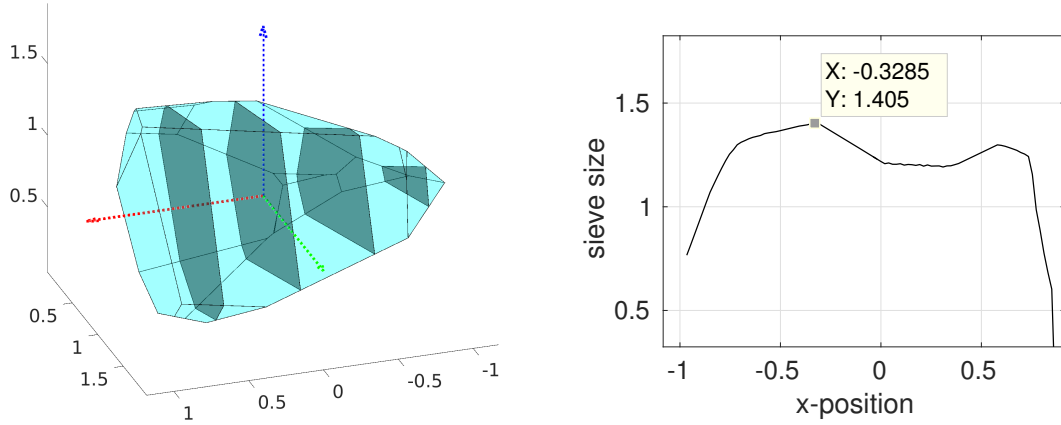
Figure 4.7: Illustration of the two possibilities of a box fitting through its sieve.

minimum area bounding rectangle, see Theorem 2 in the publication of Freeman and Shapira [66, p. 411]. As a result, it is not sufficient to rotate the polygon in discrete steps using e.g. Shamos' rotating calliper algorithm [159]. Please see figure 4.9 for a depiction of the method.

This process is then executed for an arbitrary number of slices along $\mathbf{v}_L$. Certainly, the position of the slice with maximum S is unknown. Furthermore, it is not possible to reduce the loci of slicing to certain hotspots, like the centroid. For non-convex particles, this is immediately clear. However, it is interesting to see that even for a convex polyhedron, the second derivative of the curve of S_{SLICE} over L can be positive. For the showcase VP, this is attributed to the fact that the major axis of the polygonal slices changes from alignment with y- to alignment with z-direction over the length of the particle. Also, the number of slices needs to be sufficiently high in order to achieve a reliable result for S_{SLICE} . Here, 100 equidistantly spaced slices along the length of the particle are used.

Projection along major axis

This method constitutes a simplification of the preceding one. After rotation to the global coordinate system, all nodes of the polyhedron are projected onto the y-z-plane and S_{PROJ} is computed by rotating the resulting polygon in the same manner as before. Please see figure 4.15(b).



(a) Four slices orthogonal to the major axis of a Voronoi polyhedron. Each slice has a different sieve size.

(b) S_{SLICE} along $\mathbf{v}_L$ for 100 slices.

Figure 4.8: Illustration of the slicing method for the showcase polyhedron (a). Plot of the sieve size over position on $\mathbf{v}_L$ (b).

4.3.3 Shape Index

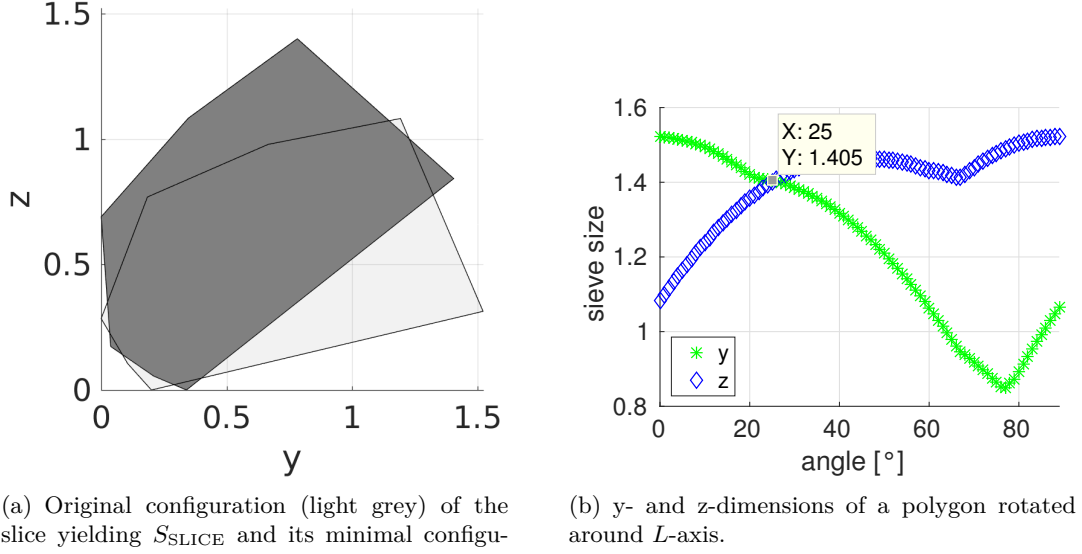
ASTM D2488 [2] addresses shape by defining elongated and/or flat particles based on their dimensional ratios. ASTM D4791 [4] uses orthogonal dimensions of the particle and a proportional calliper to classify coarse particles as flat, elongated, flat and elongated, or neither flat nor elongated. The European equivalent of these US standards is DIN EN 933-4 [19]. There, a shape index, SI , is defined which is used to classify the mineral aggregates

$$SI_3 = M_3/M_T \times 100, \quad (4.24)$$

where M_T is the total mass of sampled aggregates and M_3 is the mass of aggregates whose ratio of longest to shortest dimension exceeds 3. However, this standard does not require the dimensions to be mutually orthogonal. In Germany, the technical terms of delivery for asphalt mixes for the construction of asphalt pavements [65] require $SI_3 \leq 20$, for the top layer mixtures AC D, SMA, and MA. In the US, there is a similar requirement in the Superpave mix design guide [48]. There, no more than 10 m.% of the flat and elongated particles with ratios greater than 5:1 are admissible for asphalt pavements undergoing more than three million equivalent single axle loads in their design lives. Thus

$$SI_5 = M_5/M_T \times 100, \quad (4.25)$$

needs to be smaller than 10. Depending on the distribution of L/T , these requirements can hold true for one and the same set of particles.



(a) Original configuration (light grey) of the slice yielding S_{SLICE} and its minimal configuration shown in a darker grey.

(b) y- and z-dimensions of a polygon rotated around L -axis.

Figure 4.9: Illustration of the method to find S_{SLICE} for a showcase slice. The polygon is rotated around $\mathbf{v}_L$ in steps of 1° in figure 4.9(a). The corresponding y-, and z-dimensions are plotted versus the rotation angle in figure 4.9(b).

4.3.4 Sphericity

Sphericity, quantifies how closely a particle resembles a sphere. A widely used method to quantify this rather subjective measure was given by Wadell [173]. He defined the sphericity using surface area and volume of a given particle p . Volume can be obtained using weighing in water (Archimedes' method) for large enough particles with low water absorption or from mass if density is known. However, the surface area of irregular and/or rough particles is problematic in terms of both definition and measurement [119]. For a depiction of the fractal nature of broken rock, see e.g. Garboczi and Bullard [71, Fig. 2]. In order to further complicate matters, the “real” aggregates investigated here stem from a triangulated surface representation of CT-scanned aggregates. Therefore, the micro-roughness is already lost and the surface area is underestimated. For the aforementioned reasons Krumbein [103] proposed a different measure of sphericity, which he coined “intercept sphericity”. This measure relies only on the triaxial dimensions

$$\Psi = \sqrt[3]{\frac{WT}{L^2}}. \quad (4.26)$$

Bullard and Garboczi [42] reasoned that sphericity should be either based on the ratio of bounding spheres, or on the triaxial dimensions. Here, the latter is employed. Al-Rousan et al. [27] concluded that Krumbein's sphericity measure is well suited to differentiate between aggregates of different shape. However, Ψ cannot differentiate between shapes for which the product of W and T is similar. That means, a thin disc can have the same value of Ψ as an equiaxed rod. Therefore, already Krumbein proposed to use Ψ in conjunction with a shape classification chart established by Zingg [193]. In this chart, the aspect ratio W/L is plotted against T/W , and the diagram is divided into four quadrants. Thereby, spheres appear in the top right, discs (oblate ellipsoids) in the top left, blades (triaxial ellipsoids) in the bottom left, and rods (prolate ellipsoids) in the bottom right. Please see figure 4.12(b). There, also the aspect ratio L/T is indicated via grey areas.

4.3.5 Faceted Particles from XRCT-Scan

The data used here, originally published by Liu et al. [115], is from an XRCT-scan of SMA 13 hot mix asphalt. Details about the scanning procedure and image segmentation can be found in their publication. Voxels are isotropic with an edge length of 100 μm . Please note that the smallest particles have a larger sieve size than $\sim 2.5\text{ mm}$ for any of the used methods, c.f. figure 4.23. Hence, the image resolution is assumed to be sufficient for the reconstruction of shape and volume. This assumption is supported by an analysis in section 4.4. The data was transferred in VRML. After removing all particles which had boundary effects, 98 particles remained. The authors are convinced that a representative shape distribution is present. This position is supported by comparison of the data in table 4.1 to other researchers data, cf. [45; 42]. In contrast to the synthetic particle shape data from Voronoi tessellation, also non-convex shapes occur. A frequently used measure [85; 190; 83] for the degree of convexity is the ratio of the volume of the particle vs. the volume of the convex hull, CH , of the particle p

$$\kappa = \frac{V(p)}{V(CH(p))} . \quad (4.27)$$

The average value of κ is found to be 0.9088 for the particle set at hand, please refer to the histogram in figure 4.11(a). This mean value is quite close to the one found by He et al. [83, Fig. 7(b)] for a crushed rock of size range 0 mm to 2 mm using 2D projections. In order to get a feeling for what the degree of convexity actually means for the particle shape, two examples with a considerably distinct κ are depicted in figure 4.10.

The mean sphericity of the XRCT-scanned set is found to be $\bar{\Psi} = 0.6783$. Please note that all shape classes are present as can be seen from Zingg's diagram in figure 4.11(c).

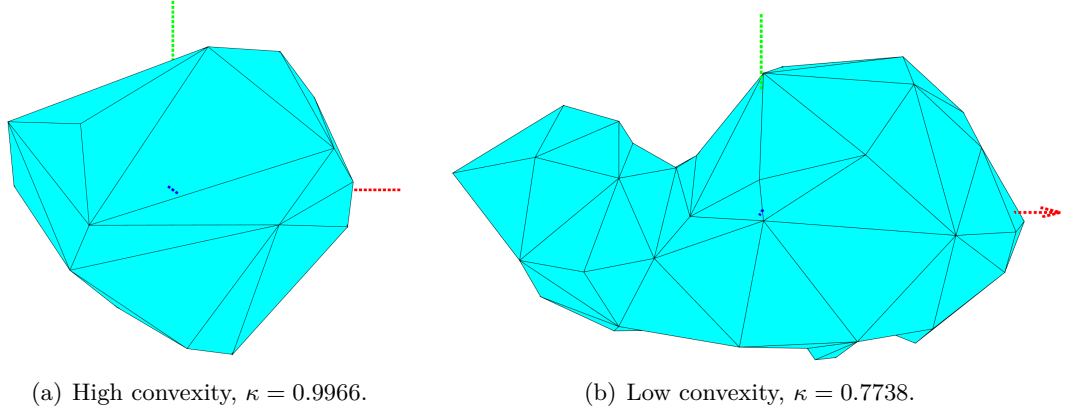


Figure 4.10: Examples of coarse aggregates with high (a), and low (b) degree of convexity κ .

$\#p$	$\bar{L}$ [mm]	$\bar{W}$ [mm]	$\bar{T}$ [mm]	$L/T > 3$ [m.%]	$L/T > 5$ [m.%]	$\bar{\Psi}$	$\bar{\kappa}$
98	10.0152	7.2171	4.3943	13.0254	0.0	0.6783	0.9088

Table 4.1: Shape parameters of the XRCT-scanned particle set.

4.3.6 Synthetic Particle Data Set

The typical methods to obtain aggregates for road construction are blasting and crushing. Garboczi and Bullard [71] concluded that particles retrieved from one and the same source exhibit a high degree of self-similarity. Voronoi polyhedra are scale invariant. In order to assess the suitability of the previously presented estimators by comparison to the slicing method, 3571 strictly convex VP are created. All computations are done in **Matlab R2015b**. The VP are generated using Matlab's implementation of **qhull** [36]. The seeds are uniformly distributed pseudorandom triplets using **rand(N,3)**, where N is the number of seeds, after initialisation using **rng('shuffle','twister')**. The mean polyhedral volume is arbitrarily chosen to be unity. In order to increase the shape heterogeneity of the polyhedra, some VP are stretched and others are compressed in x-direction while pertaining the volume (isochoric deformation). This is done using the deformation gradient tensor

$$\mathbf{F} = \begin{bmatrix} \lambda & 0 & 0 \\ 0 & \frac{1}{\sqrt{\lambda}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{\lambda}} \end{bmatrix}. \quad (4.28)$$

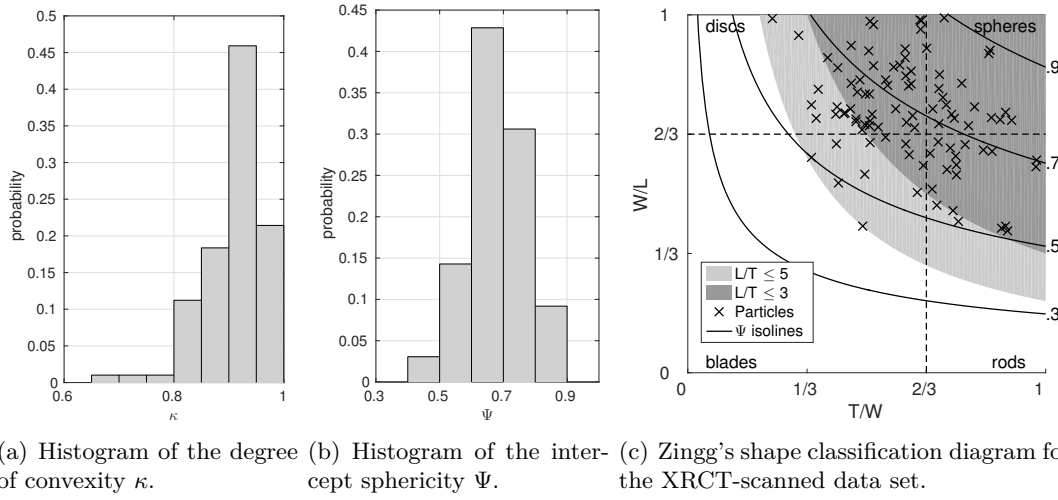


Figure 4.11: Histograms of κ (a), Ψ (b). In (c), Zingg's diagram for the 98 XRCT-scanned coarse aggregates is shown. The dark grey area highlights the regime of $L/T \leq 3$, and the bright grey area highlights the regime of $L/T \leq 5$. The curved solid lines are Krumbein's intercept sphericity isolines.

Using $\lambda > 1$, prolate particles are generated. Prolate particles are commonly perceived as “elongated”, meaning that $L > W, T$, and $W \approx T$. In contrast, oblate particles are commonly perceived as “flat”, meaning that $L \approx W$, and $L, W > T$. For the complete particle set generated $0.3 \leq \lambda \leq 2$. Please see table 4.2 for quantitative information and figure 4.12(b) for visualisation. Please note that the similarity between the histograms of Ψ of the XRCT-scanned set (figure 4.11(b)) and the synthetic set (figure 4.12(a)) is limited due to the more extremely shaped VP. However, the mean values of Ψ are almost identical.

$\#p$	$\bar{L}$	$\bar{W}$	$\bar{T}$	$L/T > 3$ [m. %]	$L/T > 5$ [m. %]	$\bar{\Psi}$
3571	2.1639	1.4308	0.9308	27.4142	5.1060	0.6740

Table 4.2: Shape parameters of the synthetic particle data set.

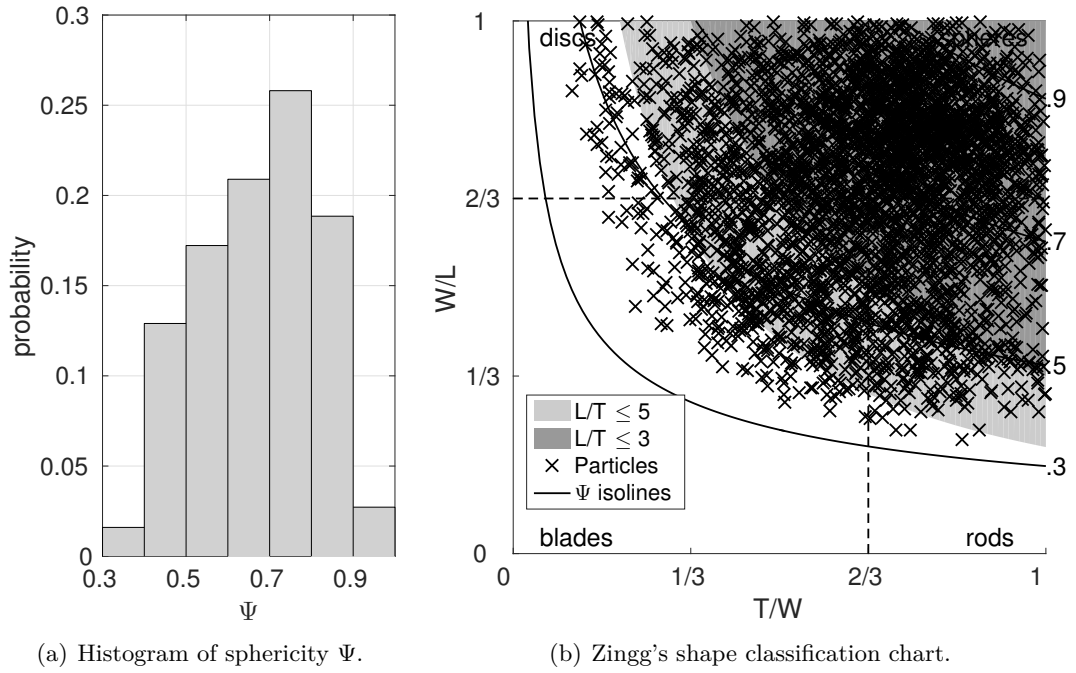


Figure 4.12: Shape characteristics of the particle set of 3571 VP. (a) shows the histogram of Ψ , and (b) shows Zingg's shape classification chart.

4.4 Voxel Size Analysis

It is undoubtedly questionable whether the XRCT resolution of $100\mu\text{m}$ used in the present study is sufficient to recreate the searched for quantities in satisfactory precision. Therefore, an attempt is made to elucidate the subject in this section. The rationale is to take particles with known properties like volume, principal axes, and thus linear dimensions and sieve sizes, obtain their voxel description and check the accuracy with which these properties can be reconstructed. However, this is not done using real particles and XRCT scanning here, but virtual particles from which pseudo XRCT data is generated. This procedure is motivated by the following reasons. It is unclear how a real particle set for verification purposes should be manufactured. It is presumably possible to 3D print particles with known properties. However, the printing process introduces additional uncertainties and the phase contrast between particles and embedding material might be insufficient for image segmentation.

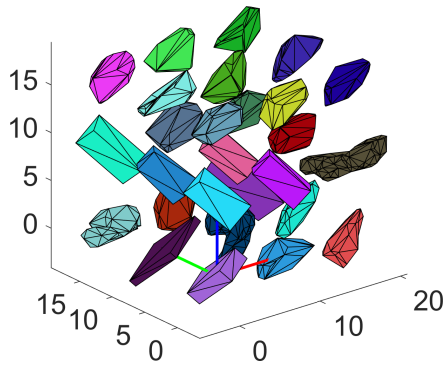
Furthermore, it is worthwhile to conduct several scans of the same sample and change its orientation and position with respect to the voxel grid between measurements. Since insufficient resolution could still accidentally (or luckily) yield rather

exact results, this is a necessary step to quantify the deviations and their diminishing with increasing resolution. To conduct such a study in reality is prohibitively costly to the authors.

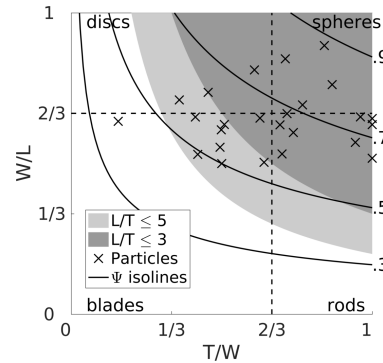
This section is organised as follows. First, the sample data set is described. Then, the employed method to create pseudo XRCT data is presented, followed by the the tools for size analysis. Then, the results are shown.

4.4.1 Sample Data Set

In order to explore the quality of reconstruction, the sample particle set is chosen to exhibit a high shape variety. Therefore, the two bricks and the showcase VP from section 4.3.1 are chosen together with three XRCT scanned particles of minimum and of maximum degree of convexity κ , respectively. This includes the particles shown in figure 4.10, which are also used in the study of mesh convergence. Furthermore, the first three² prisms and antiprisms are used. The rest of the particle data set consists of VP, deformed employing equation 4.28 using $\lambda = 3/2$. In total, there are 27 particles which are arranged in a $3 \times 3 \times 3$ grid for generation of pseudo XRCT data. The complete set is depicted in figure 4.13(a), the shape variety is highlighted through Zingg's diagram in figure 4.13(b). There, it can be seen that all shape classes are present and that Ψ varies pronouncedly.



(a) The polyhedral sample data set.



(b) Zingg's shape classification chart of the same data.

Figure 4.13: View of the tetrahedral description of the 27 particles used for the pseudo XRCT data (a), and Zingg's shape classification chart of the same data (b).

Volume reconstruction becomes more accurate with increasing particle size, which is equivalent to decreasing voxel size. Hence, the polyhedral sample data particles

²In terms of nodes of bottom and top surfaces.

are scaled to different sizes based on the **EVS**, namely 1 mm, 2 mm, 4 mm, 6 mm and 8 mm. As the **EVS** is a function of volume (cf. equation 4.17), also the volume of particles is identical for each realisation. For each size, the methodology described in section 4.3.1 is carried out using the mesh density identified in section 4.3.1. The sample data set is available for download as supplementary material.

4.4.2 Generation of Pseudo XRCT Data

As already noted in section 4.3, the voxel grid can be used directly to compute volume, principal axes and finally linear dimensions and sieve sizes. To achieve this, equation 4.2 is changed so that $\mathbf{r}_i$ simply points to the voxel center. Here, an equidistant voxel grid with voxel size $S_v = 0.1$ mm, is used. Thus, equation 4.3 is replaced by $V_i = S_v^3$.

An equidistant point grid is created whose spacing is the desired voxel size. Then, Sven Holcombe's **inpolyhedron** routine [87] is used to detect points lying inside of one of the particles. The inside points are given non-zero integer numbers unique to one particle, and the outside points are assigned zeros. For each choice of **EVS**, three pseudo XRCT data sets are generated. For each set, the voxel grid is shifted randomly by a fraction of one voxel size and the particles are rotated randomly between 0° to 89° around the z-axis.

For a visualisation of the method, please refer to figure 4.14. There, the particle from figure 4.10(b) is shown scaled to two different sizes and under different orientations.

4.4.3 Results

The mean error between the exact e.g. volume, V_e , and the reconstructed volume from voxel information, V_r , is defined as

$$\bar{\epsilon}_v = \frac{1}{3 \times 27} \sum_{s=1}^3 \sum_{p=1}^{27} \frac{|V_e^p - V_r^{ps}|}{V_e^p} \quad , \quad (4.29)$$

where s indicates the voxel data set and p is the particle. Errors of different quantities are measured in the same fashion. The errors of reconstructed volume, linear dimensions, **EVB**, and **EVE** for the chosen **EVS** of the particles are given in table 4.3. Please note that S_{PROJ} and S_{SLICE} are not given there, since these estimators require triangulation. It can be seen, that all errors diminish almost monotonously with increasing particle size. Volume reconstruction is rather accurate with an error of $\approx 0.2\%$ for particles of size 2 mm. The linear dimensions exhibit the highest mean errors among the analysed quantities. However, the sieve sizes, which are derived from the linear dimensions show smaller errors in the regime of $\approx 1\%$ for particles of size 2 mm. The authors believe that the errors are satisfactorily small for accurate shape and size

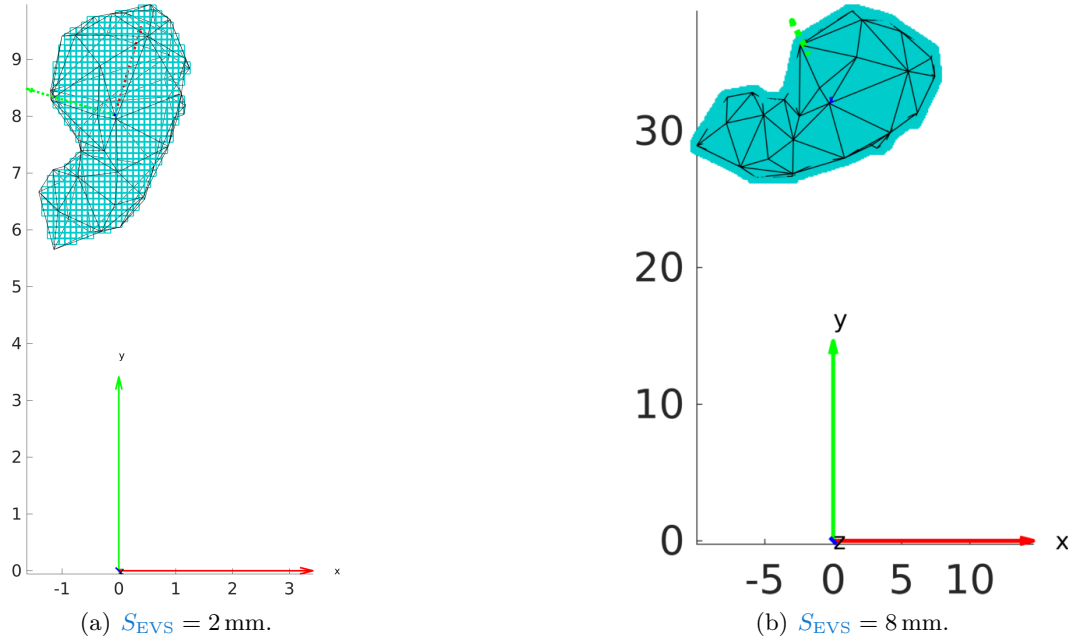


Figure 4.14: View in z-direction of the particle shown in figure 4.10(b) with inside voxels. In (a), there are 4191 voxels and in (b) there are 218862 voxels inside the particle.

analysis. Thus, a voxel size of $100\mu\text{m}$ is deemed sufficient for analysis of particles ≥ 2 mm.

4.5 Results & Discussion

4.5.1 Uniqueness of Linear Dimensions

The linear dimensions as calculated via equation 4.11 do not necessarily yield L to be the maximum distance D_{max} between any two nodes of the VP. This is immediately clear e.g. for the $4 \times 2 \times 1$ brick from section 4.3.1. There D_{max} would be the length of its space diagonal, 4.58, being 14.56% larger than $L = 4$. However, this way of measurement would be in stark contrast to typical standards [4]. This certainly unrealistic example serves illustrational purposes. Nevertheless, the problem persists as can be seen in figure 4.15. There, D_{max} is highlighted by a dashed line. Clearly, its orientation deviates strongly from $\mathbf{v}_L$. However, the authors find that their way of defining the direction in that L should be sampled more intuitive.

S_{EVS} [mm]	$\bar{\epsilon}_V$	$\bar{\epsilon}_L$	$\bar{\epsilon}_W$	$\bar{\epsilon}_T$	$\bar{\epsilon}_{EVB}$	$\bar{\epsilon}_{EVE}$
1	8.73E-03	5.66E-02	9.30E-02	9.78E-02	4.35E-02	3.04E-02
2	2.07E-03	2.31E-02	4.52E-02	5.05E-02	1.40E-02	9.37E-03
4	8.74E-04	1.16E-02	2.89E-02	3.25E-02	1.05E-02	6.30E-03
6	8.76E-04	6.98E-03	1.66E-02	2.07E-02	7.27E-03	3.26E-03
8	7.59E-04	5.27E-03	1.85E-02	2.13E-02	8.30E-03	3.97E-03

Table 4.3: Mean errors of volume, linear dimensions, and two sieve sizes for reconstruction from voxel data for differently sized particles using a voxel size of 100 μm . Three distinct pseudo voxel data sets, containing 27 particles each, have been used to calculate the errors.

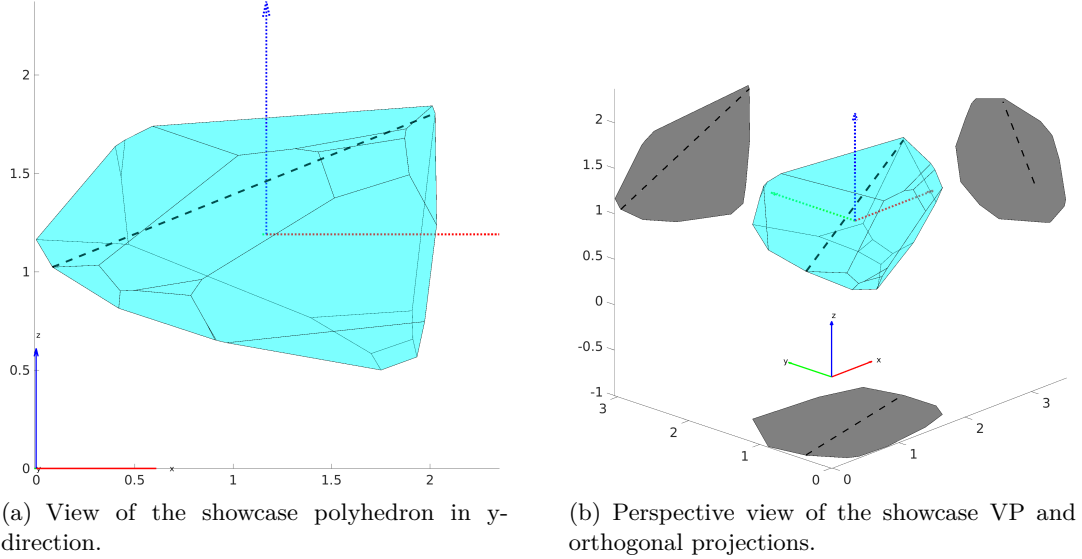


Figure 4.15: Showcase VP in projection to x-z-plane (figure 4.15(a)), and perspective view with orthogonal projections (figure 4.15(b)). The dashed lines indicates the maximum distance between any two nodes of the VP.

Certainly, there are polyhedra for which the measurement of linear dimensions is ambiguous. As Fernlund [63] expressed it: “Subjectivity for orientation of particles increases with increased particle irregularity... .” Please also see Bullard and Garboczi [42, sec. 3.2] for a discussion. For the following reason, our method does not guarantee that $L > W > T$. Imagine a flat brick with a protrusion normal to its largest facet (i.e. in direction of $\mathbf{v}_T$). If the protrusion is large enough, then $W < T$. For the synthetic VP used here, and for real world data, this problem occurs when two or

more linear dimension are rather equal, i.e. for spheres ($L \approx W \approx T$), for discs ($L \approx W$), and rods ($W \approx T$). In order to quantify the ambiguities in determining the linear dimensions from the principal axes of the inertia tensor, the percentages of VP for which L , W , and T are not in ascending order, and the ratios of the respective pairs is summarised in table 4.4. Please note that for the calculation of sieve size, except of the **EVB**, it does not matter whether $W > T$. All VP, for which L is not identified as the largest dimension are rather spherical, meaning that cross sections in arbitrary dimensions have similar sieve size.

	$L < W$	$W < T$	$L < T$
%-particles	2.2963	1.7082	0.0
mean size ratio	0.9450 ± 0.0391	0.9655 ± 0.0273	-

Table 4.4: Percentages of faulty identifications of L , W , T and their mean ratios including standard deviation.

4.5.2 Sieve Size Estimations of Synthetic Particle Data Set

For the VP data set, all sieve sizes calculated via **EDE**, **EVB**, **EVE**, **EVS**, and **PROJ** are divided by S_{SLICE} for normalisation. Then the individual values for each particle are plotted against Ψ in order to check whether estimations are influenced by sphericity, see figure 4.16.

In order to evaluate the results better, the mean values, standard deviations and slopes of trendlines of the sieve size estimators are displayed in figure 4.17.

It can be inferred from both figures, that the **EVS** exhibits the highest scatter and the worst slope. Expectably, both **EDE** and **EVE** have a similar slope, but interestingly, the **EVE** has less scatter, the best of the abstract shape estimators. Both scale well with Ψ . The **EVB** has the second highest scatter, but it also scales satisfactorily with Ψ . Unsurprisingly, S_{PROJ} does never underestimate S_{SLICE} , whereas all abstract shape based estimators can over- or underestimate. In summary, the abstract shape based estimators are ranked in terms of scatter: **EVE**, **EDE**, **EVB**, and **EVS** (from best to worst). In terms of scaling with Ψ , the ranking is **EDE**, **EVE**, **EVB**, and **EVS**. However, the first three are all close and the **EVS** comes fourth by a big margin in both cases.

In order to check whether the statistics are robust with respect to sample size, two smaller data sets are created. The results are sorted by volume to introduce randomisation and then every 3rd, or every 9th particle is picked resulting in a mid-sized set of 1191 VP and a small set of 397 VP. The results are shown in figure 4.18. There are hardly any susceptible changes to the means and standard deviations. The slopes experience the strongest changes, but all signs are retained. Particularly, the

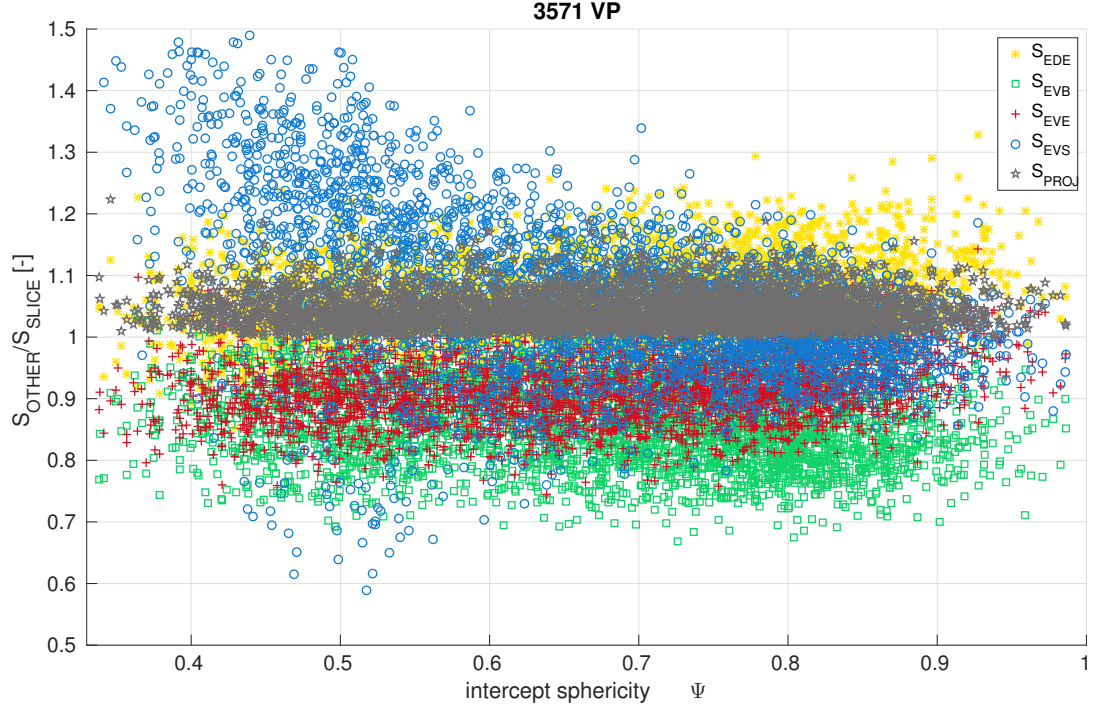


Figure 4.16: Sieve sizes of VP from different estimators, normalised by S_{SLICE} and plotted against Ψ .

ranking order is kept. Therefore, it is concluded that the set of 3571 VP is statistically representative.

Due to aforementioned faulty identification of L , W , and T , see section 4.5.1, it is furthermore checked whether excluding the faulty results impacts the results. 4% of all VP were excluded and the mean values and trends computed again, see figure 4.19. It is concluded that there is no pronounced impact on the results. It has to be kept in mind, though, that it is only possible to exclude the VP, which have L , W , and T *not* in descending order. VP, for which L , W , and T were erroneously computed to be ordered could not be identified.

Sieve Size Estimations for Zingg's Shape Classes

In order to further explore the suitability of the sieve size estimators, the complete VP data set is divided into the four shape classes according to Zingg, cf. figure 4.12(b). Trends and mean values are shown in figure 4.20. Again, PROJ delivers the best predictions. Of the abstract shape based estimators, the **EVE** consistently exhibits the lowest scatter, thereby confirming the result for the complete data set. For blades

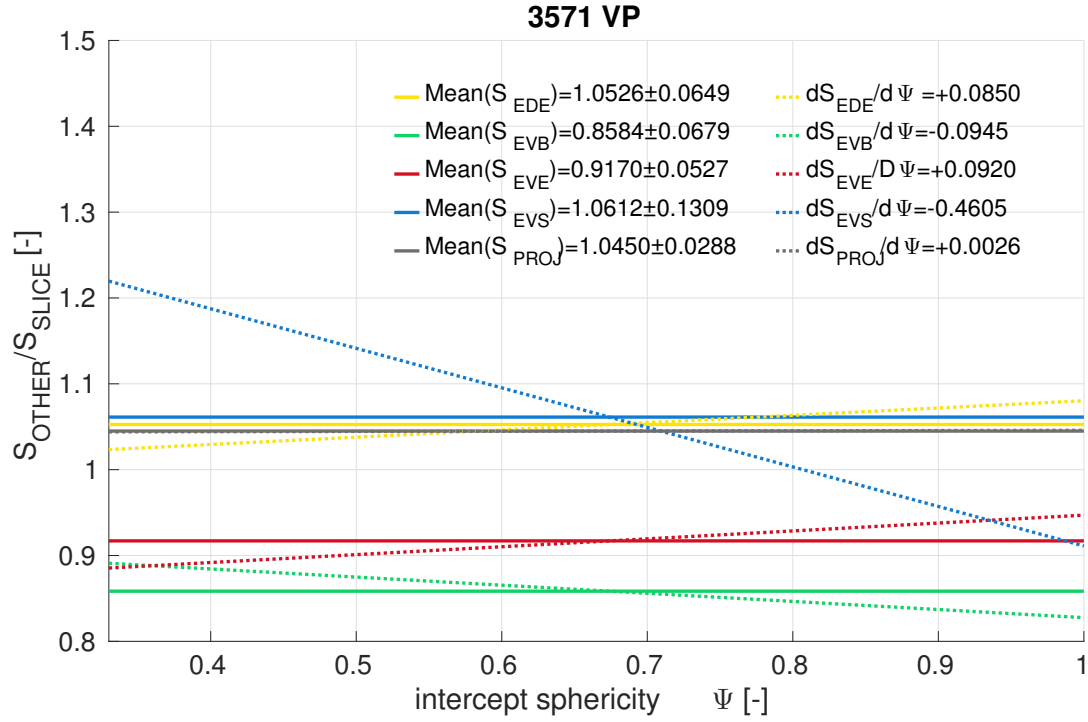


Figure 4.17: Mean values of relative sieve size, standard deviations, and slopes of the individual values shown in figure 4.16.

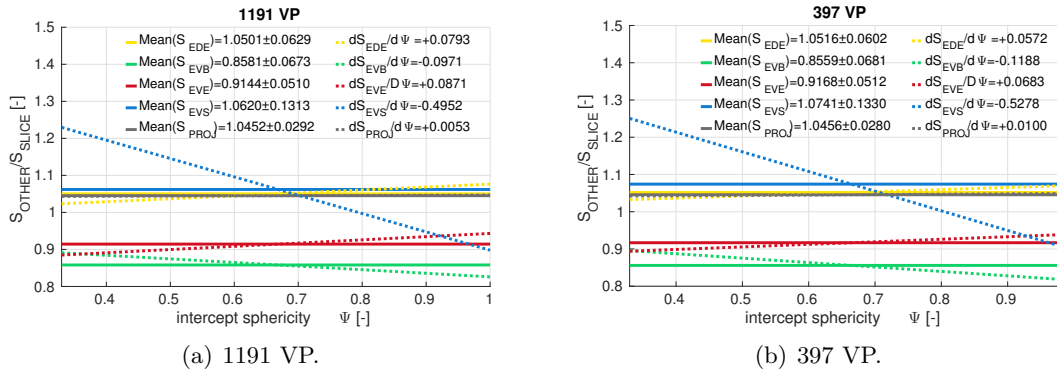


Figure 4.18: Mean values of relative sieve size, standard deviations, and slopes of the individual values for 1140 VP (a), and 397 VP (b).

and rods, the **EVE** exhibits the smallest slope, too. For spheres and discs, the **EVB** scales best with Ψ . However, there is a problem with the **EVB** as its mean for spheres

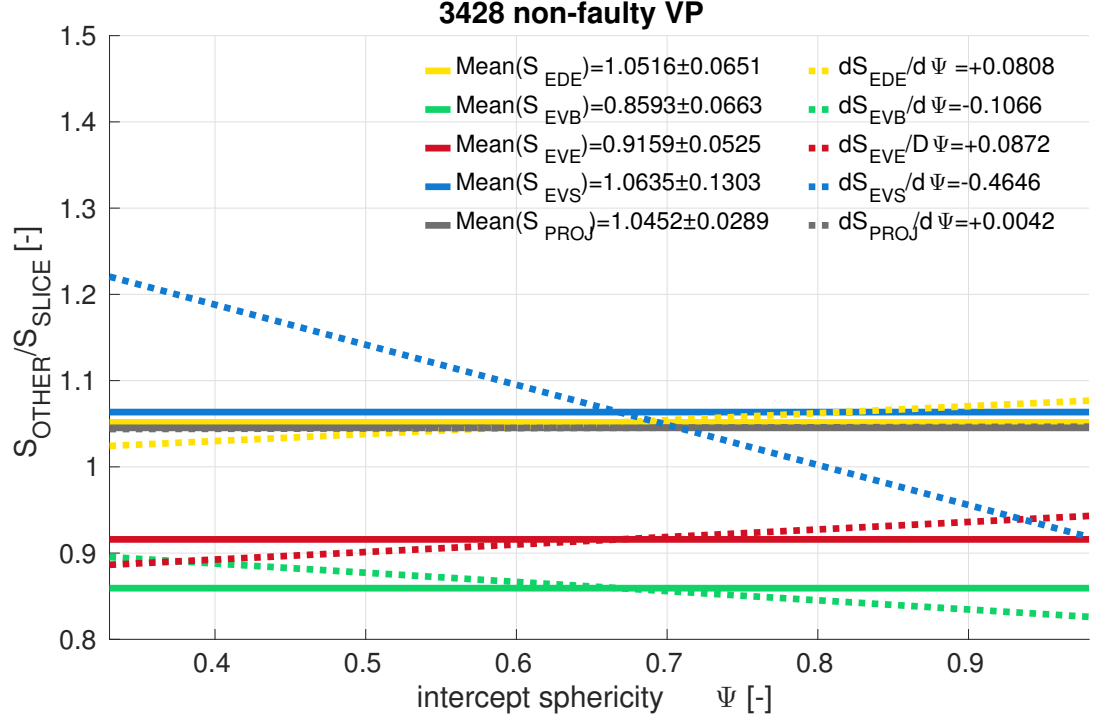


Figure 4.19: Mean values of relative sieve size, standard deviations, and slopes of the 3428 non-faulty VP from the complete set shown in figure 4.16.

and rods is significantly lower than for discs and blades. As a result, the deviation of the mean sieve size of the EVB from S_{SLICE} cannot be compensated by a constant factor. The EDE has similar trends to the EVE, which does not surprise since one is derived from the other through isotropic scaling. The EVS has both the worst standard deviations and trendlines. Even for spherical shapes, it is outperformed by most other estimators, only the EDE exhibits a higher scatter. Strikingly, it is not even possible to compensate the EVS for deviations from the mean with a constant factor since its mean underestimates the sieve size of discs, but overestimates all other shape classes. All other estimator's means consistently over- or underestimate S_{SLICE} . The striking changes in the scaling behaviour of the EVS with Ψ can be explained as follows. For rods, both W and T are smaller than the diameter of the EVS which thus overestimates S . For blades, $S_{\text{EVS}} \approx W$, but blades fit diagonally through a square aperture, cf. figure 4.6. For discs, usually $S_{\text{EVS}} < W$, which becomes more pronounced when Ψ decreases, i.e. the thickness decreases relatively to the other dimensions. For spheres, combinations of all these cases are present, hence simple conclusions cannot be drawn.

In summary, the **EVB** and **EVE** exhibit the best scaling with Ψ , and the **EVE** exhibits the smallest scatter of the abstract shape based estimators. The **EVS** should be abandoned.

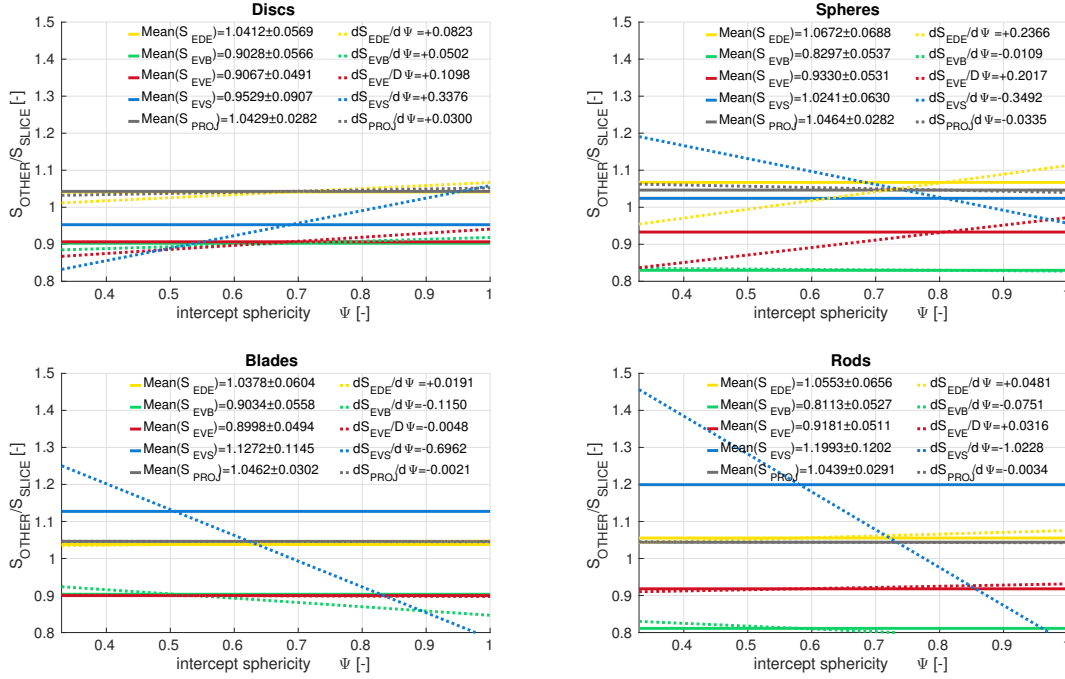


Figure 4.20: Trends and mean values of the complete VP data set divided into the four shape classes according to Zingg.

4.5.3 Sieve Size Estimations for XRCT-scanned Particles

The major difference between the XRCT-scanned and the synthetic data is the lack of convexity of VP. In order to evaluate the impact of not strictly convex shapes, the previous analysis is also conducted for the 98 scanned particles. In the same manner as before, the relative sieve sizes $\frac{S_{OTHER}}{S_{SLICE}}$ are plotted against Ψ in figure 4.21. Trends, mean values, and standard deviations are shown in figure 4.22. Here, the best result of the simple estimators is given again by the **EVE**, with the smallest slope of the trendline and the smallest scatter. As before, the **EVS** does not scale well with Ψ . In general, all results are rather similar to the ones of the synthetic data set, c.f. figure 4.17.

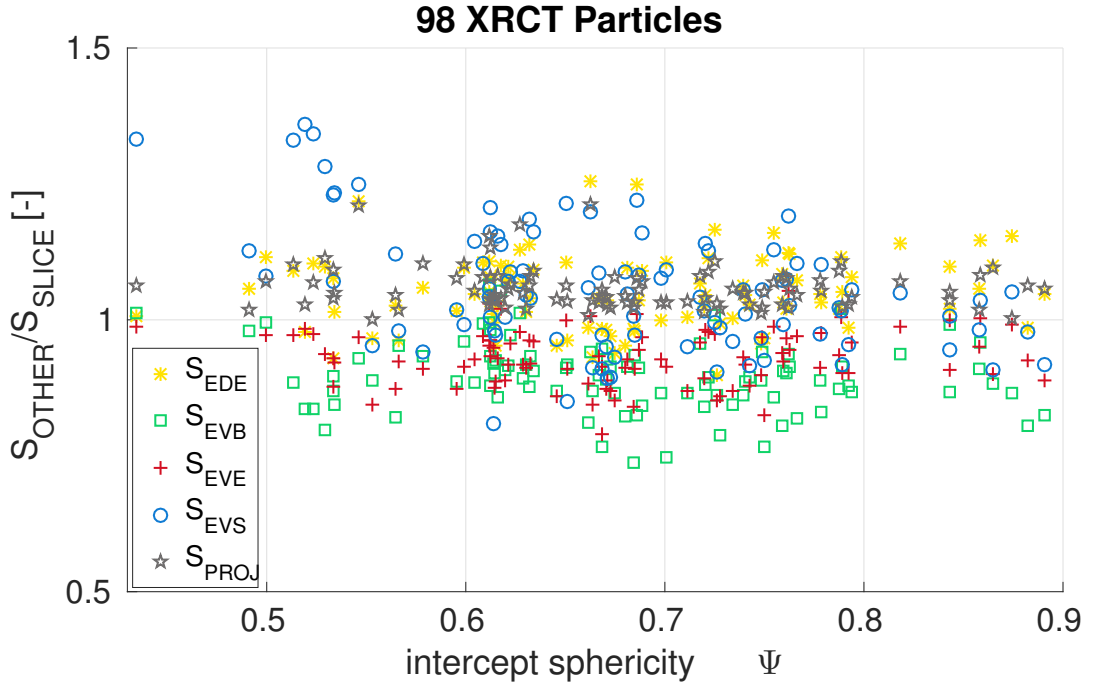


Figure 4.21: Sieve sizes of XRCT-scanned particles from different estimators, normalised by S_{SLICE} and plotted against Ψ .

4.5.4 Influence of Sieve Size Estimators on Granulometric Curves

Particulate materials are susceptible to changes in their particle size distribution. Hence, it is worthwhile to control the particle size and the size distribution as accurately as possible. In road engineering, it is common practice to plot the cumulative mass³ percentage of aggregates against the sieve size. In figure 4.23, such a diagram is presented using S as given by all estimators for the XRCT-scanned particles. Here, the results are sorted by, but not normalised by S_{SLICE} , which makes the absolute sieve sizes of small particles appear to be closer together, although their relative differences are similar. The absolute differences in sieve size prediction are striking. The largest particle is identified consistently by all estimators except of S_{PROJ} . For this particle, $S_{EVB} = 9.51$ mm, but the EVS predicts a value of 12.1 mm. One could draw the conclusion from looking at figure 4.23 that no simple shape estimator performs significantly better than the EVS . However, this is because the mean values of the estimators have not been compensated for deviations from S_{SLICE} . In figure 4.24, this

³Again, mass density $\rho = 1$.

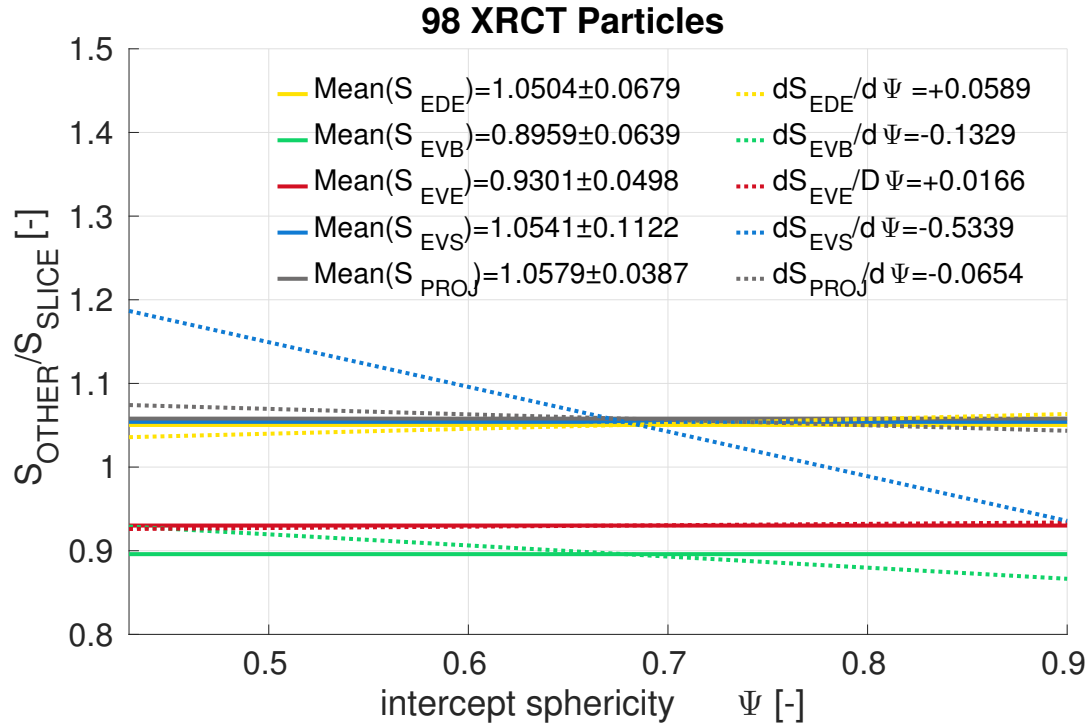


Figure 4.22: Individual results and trends of 98 XRCT-scanned coarse aggregates.

compensation has been applied. There, it can be perceived, that the scatter in the estimates by the **EVB**, and particularly by the **EVE** are smaller than by the **EVS**.

4.6 Conclusions & Outlook

Under the assumption that slicing delivers the most accurate results, all abstract shape based sieve size estimators are biased. The **equivalent volume ellipsoid (EVE)** is a strong contender which has less computational cost than the slice, or projection based methods. Its standard deviation is $\approx 5.3\%$ for the Voronoi polyhedra, and $sd \approx 5.0\%$ for the XRCT data. The **equivalent volume box (EVB)** is also strong with an $sd \approx 6.8\%$ for the Voronoi polyhedra, and $sd \approx 6.4\%$ for the XRCT data. The real difference between the two is only revealed when individual shape classes are considered. The **EVE** excels in scaling behaviour with sphericity for blades and rods. For spheres and discs, the **EVB** scales better. However, the **EVB** suffers from its variable mean. Based on the present findings, the **equivalent volume sphere** should be abandoned. It is proposed to employ either the **EVE** or the **EVB** and compensate for their consistent underestimation using a constant factor. It is judged that no advantage

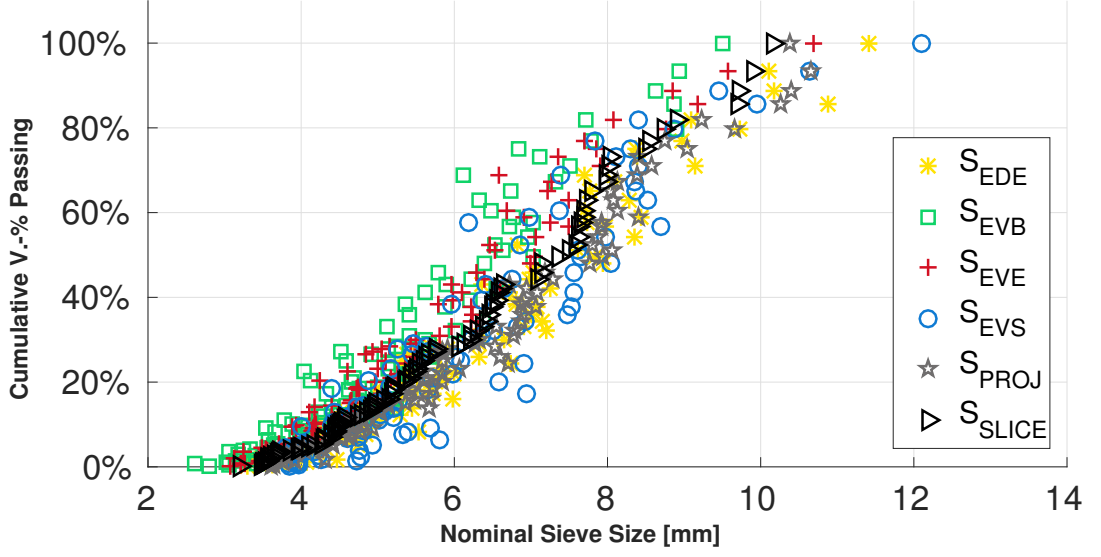


Figure 4.23: Cumulative distribution of the XRCT-scanned data set using different sieve size estimators. Please note that only S_{SLICE} has been sorted in ascending order from left to right. The results of S_{OTHER} are shown in the same order as S_{SLICE} . Hence, the results for one and the same particle appear in the same y-position.

can be gained from using the [equivalent dimension ellipsoid](#). However, when precision is critical, slicing or a compensated projection method should be used.

Furthermore, it is necessary to look at relative errors due to the reasons given in section 4.5.4. The differences in sieve size estimation can lead to the situation that a particle size distribution that adheres to the bounds of a certain standard given one particular estimator, is found to be violating the bounds when a different estimator is used.

While the statistical relevance of the synthetic data set has been investigated, it is questionably if the XRCT-scanned set is large enough. Although similar means and trends were found, some caution in extrapolating the results is required. Furthermore, it is not clear how the non-convexity influences the results of S_{SLICE} , which is used as a reference measure here. While the two example aggregates shown in figure 4.10 most likely pass in the direction of $\mathbf{v}_L$, this need not hold true in general. Further research in that direction could use simulated annealing in order to create non-convex synthetic particle data. Then, S_{SLICE} could be established orthogonal to the medial axis, which is closely linked to the Voronoi tessellation [112; 30], instead of the first principal axis.

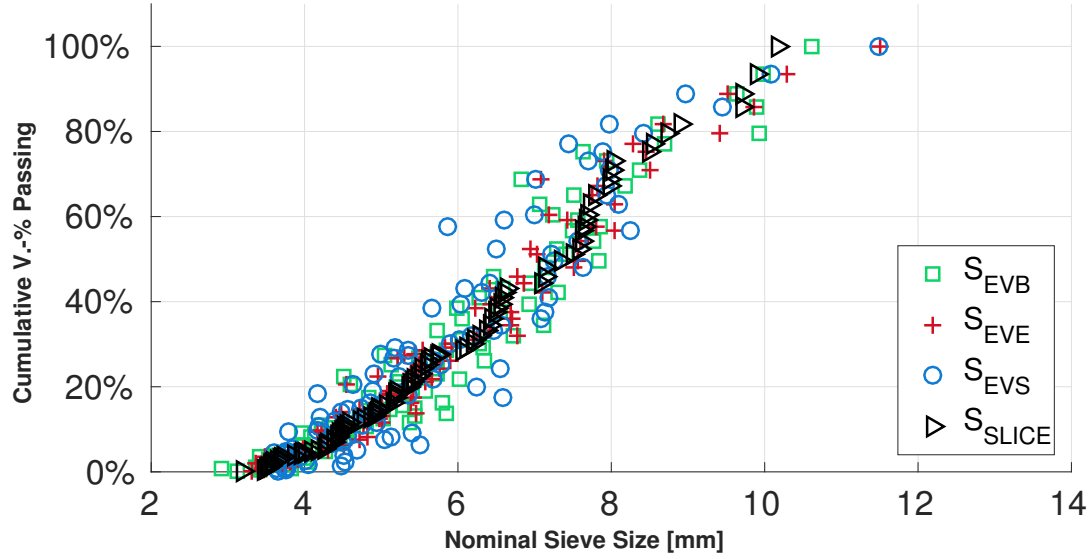


Figure 4.24: Cumulative distribution of the XRCT-scanned data set using S_{EVS} , S_{EVE} and S_{EVB} with their mean deviations from S_{SLICE} scaled to unity. The same order as in figure 4.23 applies.

Synthetic 3D models of asphalt concrete can only be meaningful if the grains are accurately modelled. It is concluded that VP can cover a wide range of shapes typically encountered in coarse aggregate for road construction. Therefore, VP offer a promising synthetic alternative to image data. However, it is not yet known to what extent the strict convexity of particles from a Voronoi tessellation influences e.g. mechanical properties.

Acknowledgements

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5 Additional Investigations

The results of additional investigations, which extend the results given in the three publications, will be given here. Parts of the research have been published previously in a proceedings [134], while some of the results have not been published, yet.

The first analysis deals with the suitability of virtual particles from the nested VT algorithm to represent real particles, see section 5.1. The effect of the SSA on reinforcement in composites, which was addressed in section 3.6.2, will be discussed again in section 5.3. After publication of the work presented in section 3, two inconsistencies have been discovered, which shall be addressed in section 5.2.

5.1 Validation of Morphology of Particles from Nested Tessellation

Although morphologies of VPs and XRCT-scanned particles have been compared in section 4.3.5 and section 4.3.6, it has not been done for particles from the nested tessellation algorithm described in section 3.4.3. figure 5.1(a) shows the histogram of Ψ and figure 5.1(b) depicts Zingg’s shape classification chart for 129 particles in a PSD of SMA 13, which have been generated synthetically using nested VT. Please compare these to figure 4.11(b) and figure 4.11(c). Furthermore, table 5.1 juxtaposes mean sphericities and mean shape indices from table 4.1 to the new values. The high similarity is striking.

The agreement of synthetic and real data leads to the conclusion that the nested VT does not change the morphology of the grains unfavorably, and is therefore well suited for the generation of virtual geometries of asphalt.

Data source	$\bar{\Psi}$ [-]	SI [m.%]
synthetic SMA 13	0.6658	12.44
XRCT SMA 13	0.6783	13.0254

Table 5.1: Comparison of sphericity and shape index between synthetic and XRCT-scanned data of SMA 13.

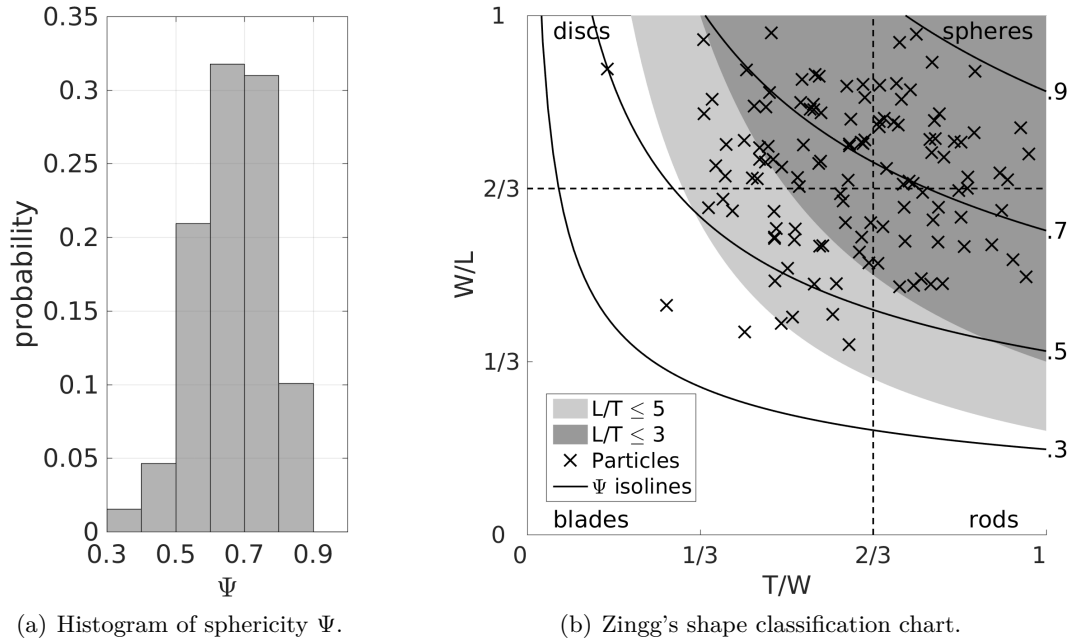


Figure 5.1: Shape characteristics of a particle set of 129 VP from a PSD of SMA 13. (a) shows the histogram of Ψ , and (b) shows Zingg's shape classification chart.

5.2 Mortar Design and Parameters Revisited — Macroscale Validation

The mortar tested in section 3.3.1 is too soft because it contained too much bitumen for a realistic representation. The mortar design assumed that the mortar is obtained when the coarse aggregates, i.e. all grains ≤ 2 mm, are taken out of the mix, while neglecting voids. See figure 5.2 for an illustration of the volumetric composition. However, it was not respected that larger grains absorb and adsorb bitumen, which in effect reduces the amount of bitumen in the mortar. The relevant literature has started to address this issue recently [171; 98; 79]. However, there is ongoing debate about the state in which the mortar exists in asphalt mixes.

Furthermore, there is an issue with the parameters of the generalised Maxwell model calibrated to the mortar data in section 3.3.2. The fit was performed using frequency defined via [cycles/time]. Although the parameters shown in table 3.2 are correct, these parameters have been used in *Abaqus* in a wrong fashion. *Abaqus* assumes, that frequency is defined as [radians/time], being higher by a factor of 2π . Hence, either the moduli, g_i , need to be divided, or the relaxation times need to be multiplied by

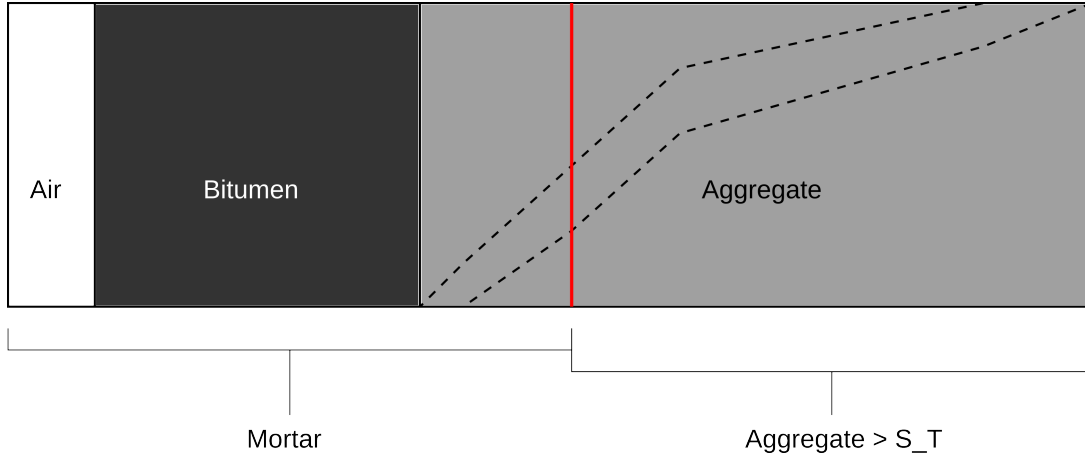


Figure 5.2: Mortar mix design according used in section 3.3.1. The red line indicates the size threshold, S_T .

2π when used in **Abaqus**. This had not been done previously. Further details about the use of Prony series parameters in **Abaqus** are presented in section 7.1.

These two issues remained unnoticed in the results shown in section 3.6, because the effects largely cancel each other out. This can be seen in figure 5.3 where experimental data of master curves of several different asphalt mixes [77; 55; 50; 98; 171] are contrasted to the simulation results from Neumann et al. [132, section 3.6]. Where necessary, the data has been shifted to a common reference temperature of 20 °C using the WLF-equation and converted from E^* to G^* assuming $\nu = 0.35$. It can be seen, that the original numerical predictions are on the soft side of the spectrum of the experimental data, but still sensible.

A comparison of the predicted moduli to experimental data had not been done in section 3.6, because macroscale data for the mix, upon which the mortar is based, was not available. To the author’s best knowledge, this still holds. Due to the fact that the parameters had been fed into **Abaqus** in a wrong fashion, the fact that the mortar moduli and hence the predicted moduli were unusually low, went unnoticed.

However, when additional investigations revealed the input error for **Abaqus**, it was also found that mortar design suffered from the discussed shortcomings. table 3.5 gives a mean value of the predicted shear modulus for the pure 9.2 mm VT of 591.87 MPa. This value is shown in figure 5.3 by a blue square and again in figure 5.4 by a black triangle. Once it is correctly respected that **Abaqus** expects relaxation times as [radians/time], that value drops to below 100 MPa a frequency of 1 Hz, shown by the black diamond markers in figure 5.4.

The Steady-State Dynamics (SSD) method mentioned in figure 5.4 is a linear perturbation method which provides the steady-state amplitude (modulus) and phase

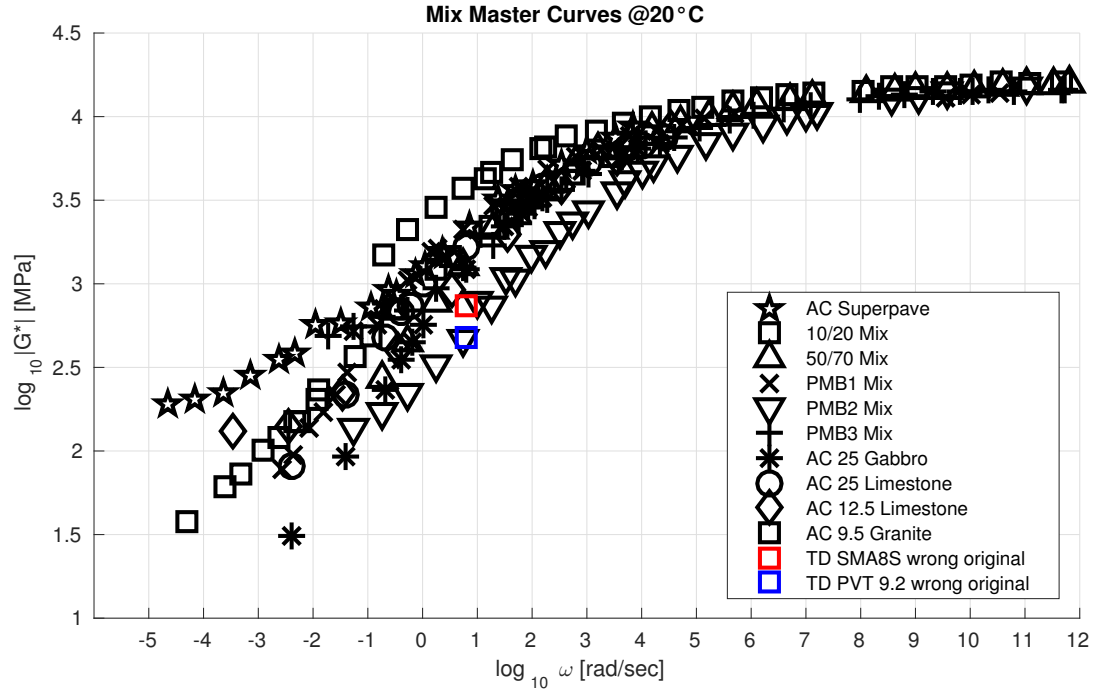


Figure 5.3: Experimental data of master curves of several different asphalt mixes taken and modified from [77; 55; 50; 98; 171] shown in black and the simulation results from Neumann et al. [132] shown in red and blue.

(loss angle) of the response of a system due to harmonic excitation at isolated frequencies. It circumvents the computation of several cycles until a steady state has been reached in time domain. Thus, this method is way faster. It is preferred over mode-based or subspace-based steady-state dynamics if significant material damping is present, which is the case here. The corresponding lines for the step definition of logarithmically distributed frequencies (default setting) in the *Abaqus* input-file read as follows:

```
*Steady State Dynamics, direct, friction damping=NO,
frequency scale=logarithmic
1e-5, 1e+2, 8, 1.
```

Here, frequencies are given as [cycles/time]. The first two numbers are the lower and upper bounding frequencies. The third number is the total number of frequency points, which includes the bounding frequencies. The fourth number is the so-called bias parameter, which can be used for closer spacing of the frequency points either toward the middle or toward the ends of each frequency interval. Here, it is unused.

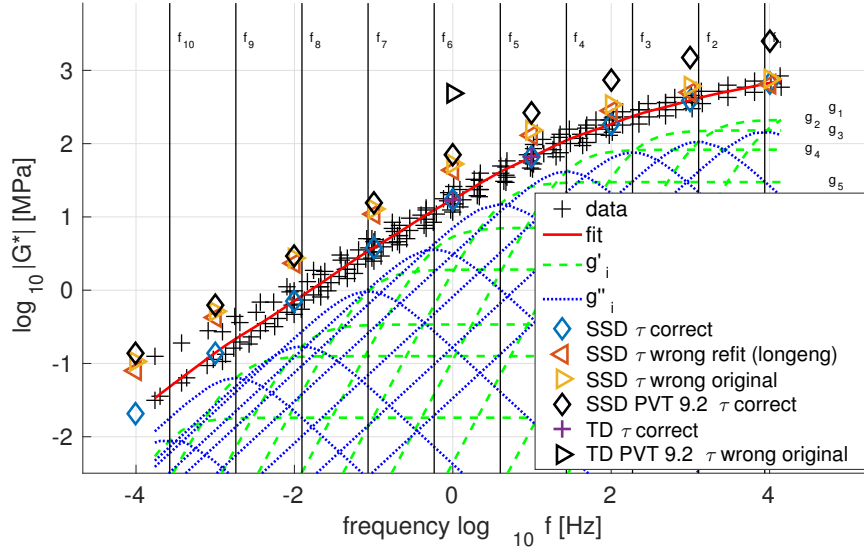


Figure 5.4: An extended version of figure 3.7 showing additional sanity checks and results from upscaling.

In order to perform sanity checks, the response of pure mortar was calculated. The result is given by the blue diamond markers in figure 5.4. For comparison, the response was also calculated in time domain, indicated by purple crosses. The results are indistinguishable. Beforehand, the pure mortar response was either given by the orange left pointing triangles, or by the yellow right pointing triangles, depending on whether the `longEng` format was used in `Matlab` to export the Prony series moduli, cf. section 7.1.

These results indicate that the mortar is now represented correctly, albeit still suffering from improper design. Hence, it remains to be determined, whether the upscaling procedure is able to deliver realistic results using presumably better mortar data.

There are only few publications available which provide experimental data for the mix and for corresponding mortars, while reducing the amount of bitumen in the mortar to lower levels in order to take absorbed and adsorbed binder into account. table 5.2 lists the compositions of some of those mortars, together with the composition used by the author. The lower bitumen content is evident, although there is no consensus of the correct value. The same holds for the void content of mortar.

The experimental data is visualised in figure 5.5. There, it can be seen, that the mortar used in section 3 is softer than the other mortars shown in table 5.2. It is even softer than the 20/30 bitumen with filler by Schüller et al. [157]. If this is a result of the different experimental designs, or simply highlighting that a 20/30 bitumen is much harder than the PMB 25/55-55A used by the author is not known.

bitumen [m.%]	fibres [m.%]	voids [v.%]	aggregate [m.%]	reference
21.1 (PmB 25/55-55A)	1	-	77.9 (limestone & diabase)	NSR17 [132]
8 (PG 64-28)	-	1 & 5	92 (limestone)	KKL15 [98]
8.27 & 11.2 (?)	-	9.1	91.73 & 88.8 (granite)	UK13 [171]
12.9 (PG 64-22 & 76-16)	-	6	87.1 (?)	GU15 [79]

Table 5.2: Different mortar compositions.

In the following, data of presumably realistic mortar compositions are used to predict the macro response and compare it to macroscale data. During upscaling, it is worthwhile to use PSDs that correspond to the mortar designs for macroscale predictions. However, it was not possible to generate geometries for the mix by Karki et al. [98], due to the small size threshold of 1.18 mm and the unfavorable PSD. Both led to a prohibitive amount of small particles. However, it was possible to generate geometries for the data by Underwood and Kim [171]. The corresponding PSD has been taken from Allen Cooley, Jr. et al. [29]. It is depicted in figure 5.6.

Underwood and Kim [171] produced mortars with two different bitumen contents, CFL-9 with low, and CFH-9 with high content, cf. table 5.2. Using CFL-9 leads to higher mix stiffness predictions than the experimental mix data given. However, CFH-9 lead to good agreement, as can be seen in figure 5.7. Please note, that upscaling has been performed at 15 °C here, since this is the reference temperature used by Underwood and Kim [171] and it was desirable to eliminate additional uncertainties. Also note that mix data has been converted from $|E^*|$ to $|G^*|$ using $\nu = 0.35$ and that five samples with three shear modes each have been used for macroscale prediction. The agreement between the prediction and mix data is satisfying.

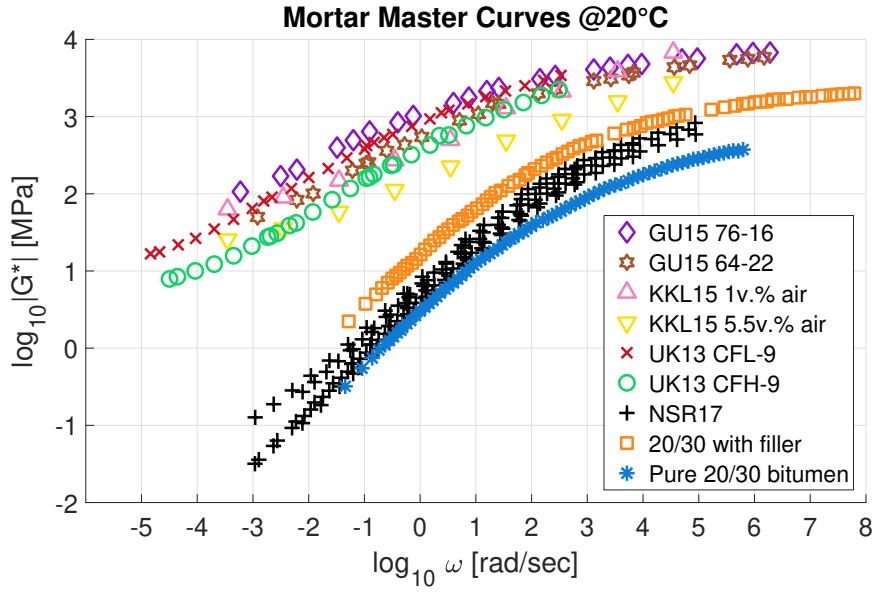


Figure 5.5: Complex shear moduli $|G^*|$ over angular frequency ω of the data available in the references given in table 5.2. Additionally, data from Schüller et al. [156] (pure 20/30) and Schüller et al. [157] (20/30 with filler) are shown. Where applicable, the data has been shifted to a common reference temperature of 20 °C.

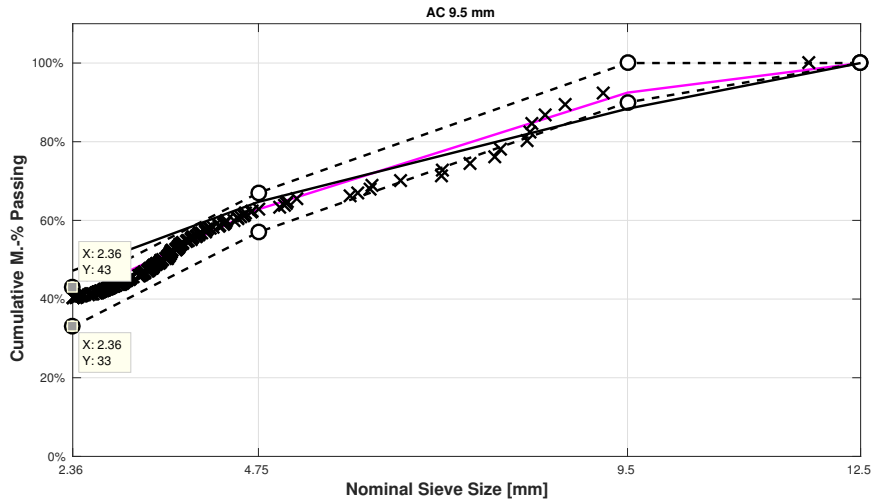


Figure 5.6: Particle size distribution of an asphalt concrete with NMAS of 9.5 mm. Data taken from Allen Cooley, Jr. et al. [29].

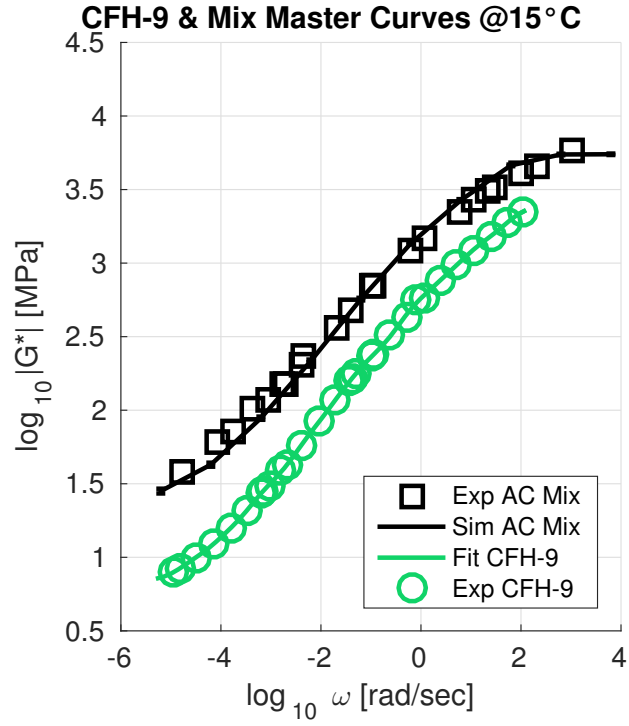


Figure 5.7: Results of the upscaling process for CFH-9. Green indicates mortar, and black indicates mix. Box and circle markers indicate experimental data by Underwood and Kim [171].

5.3 Reinforcement and Specific Surface Area

It is postulated in section 3.6.2 that the PSD, particularly the volume specific surface area, or SSA, is the reason for the differences in the effective properties. However, additional investigations have failed to provide evidence for this claim.

The statement was based on the fact that the homogenisation results of the PVT with 9.2 mm NMA exhibited lower moduli and higher loss angles than those of the 4.8 mm geometries, see table 3.5. However, after publication, it was remarked¹, that these differences are probably mesh related.

In order to investigate this issue further, a simple model was created. The principal idea is illustrated in figure 5.8. There, the large central geometry is reducible, which means that it is made of a smaller RUC shown on the left. There is no additional information contained in a reducible geometry, thus, homogenisation of the left, and of the central geometry yields the same results. Furthermore, the “window” of the unit cell can be moved around the larger reducible geometry without affecting the results using PBCs, and any multiple of the RUC can be chosen [182]. Furthermore, the dimensions of the RUC do not matter, the choice of the lengths A and B in figure 5.8 is completely arbitrary. This means that the geometry on the right delivers the same response as its magnification in the central one. Consequently, the response of the left and the right geometry is also identical.

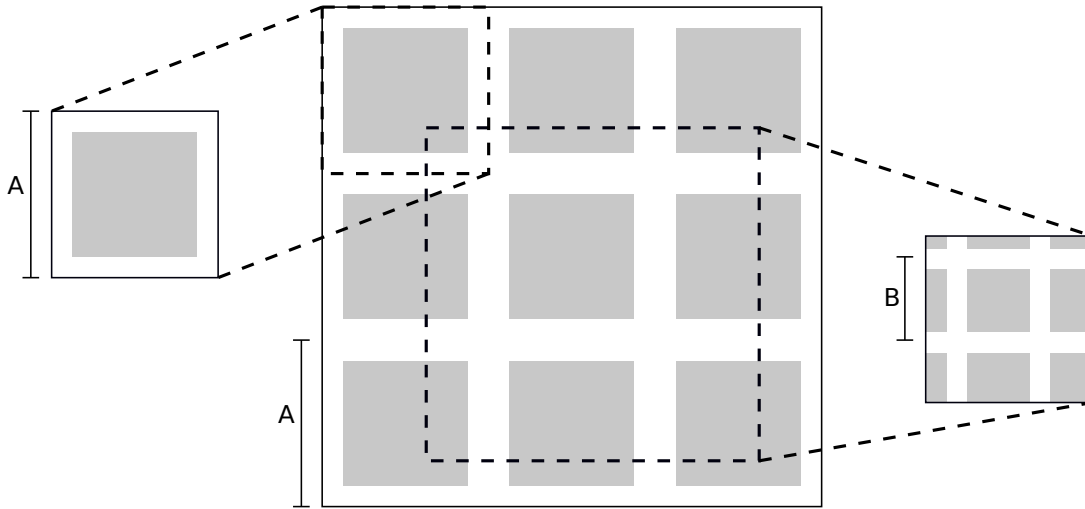


Figure 5.8: Several possibilities to define RUCs and multiples thereof from the same microstructure. All shown possibilities yield the same macro response under PBCs.

¹Thanks to Prof. Stefan Wulfinhoff for the constructive criticism.

Hence, it becomes clear that the concept of a SSA is useless in the context of self-similar RVEs. Since the response is scale invariant, it cannot depend on the SSA. The two geometries shown in figure 5.9 have been created which feature the same volume fraction², but different specific surface areas. The grey volume is linear elastic with a Young's modulus of 50 000 MPa and a Poisson ratio of 0.2. The green volume is linear viscoelastic with an equilibrium modulus of 10 MPa, an instantaneous modulus of 5000 MPa and a single relaxation time of 1 s. Its Poisson ratio is 0.35. The element size has been kept constant, i.e. finite elements in the right geometry are only have the size of the ones in the left geometry.

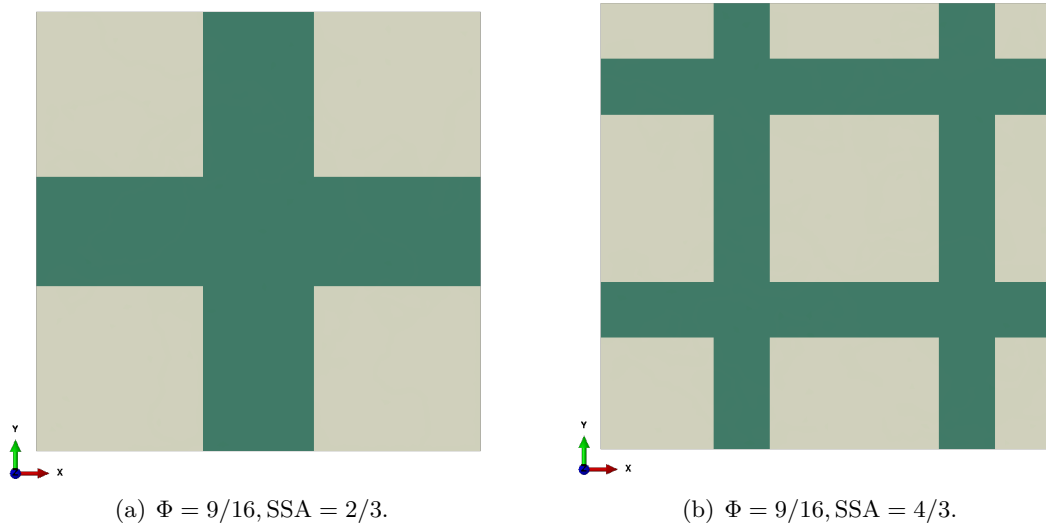


Figure 5.9: Geometries for analysis of influence of SSA on macro properties.

It was found, that there is no significant difference in the homogenised response. Moreover, the subtle differences, see figure 5.10, are likely to be a result of problems with the boundary conditions. Therefore, next to **Abaqus**, also **FEAP** was used for the computations³. There, no differences have been found.

These results probably indicate that using smaller reinforcing inclusions of the same bulk volume does not change the effective properties. Nevertheless, there can be substantial differences in the reinforcing properties between different particle sizes in reality, which are a result of the physics and chemistry at the interface. An example of this type of behaviour can be found in filled rubber, whose effective properties depend on the surface area, and surface activity of the filler [123; 111]. Furthermore, changing particle morphology, and thus necessarily the SSA of every particle without

²As these are 2D geometries, it is actually a area fraction, but the 3D terminology is adopted.

³Thanks to Lei Zhou

changing particle volume also influences bulk properties. For example, Stefanou et al. [160] report a pronounced influence of the SSA of one single inclusion on bulk properties. Importantly, the different particles are not self-similar. There, the homogenised response becomes stiffer with increasing SSA of the reinforcing phase.

Thus, it is concluded here, that changing the inclusion size while keeping the total volume fraction of inclusions constant does not influence bulk properties, as long as interface effects are not taken into account. Changing the inclusion size from 9.2 mm to 4.8 mm in must not change the response and is attributed to insufficient mesh density. However, morphology and topology do influence the macro properties, and it is thus necessary to reproduce the particle size and particle shape distributions accurately in a model.

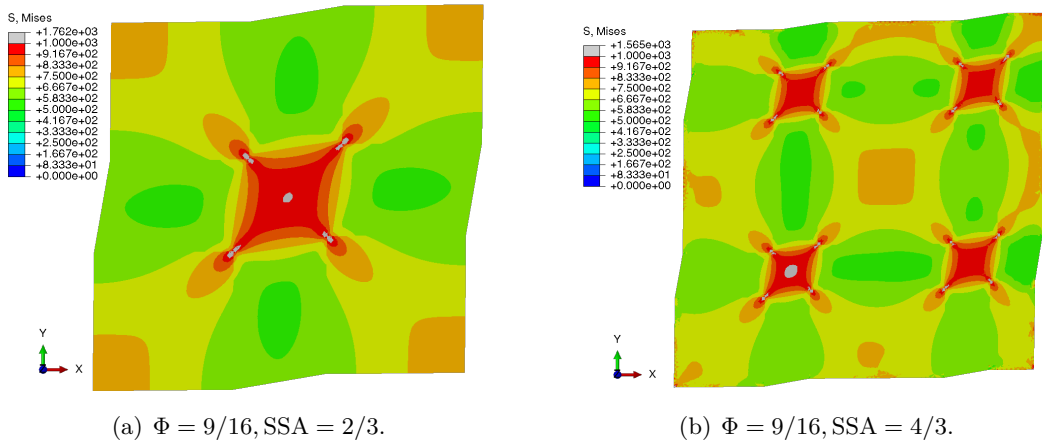


Figure 5.10: Von Mises stresses in the test geometries shown in figure 5.9. The differences in the stress field of the four RUCs in figure 5.10(b) are attributed to problems with the boundary conditions.

6 Overarching Conclusions & Outlook

A mesoscale framework for asphalt has been developed which allows to make predictions of the macroscale behaviour of bulk asphalt, but can likewise be used for detailed investigations on the smaller scale. The employed first-order strain driven homogenisation scheme is deemed sufficient for future analyses, since deformations in asphalt under traffic loading are small and only add up over time to eventually large deformations. Also damage modelling should, at least for its onset, be sufficiently accurate using small strains. Top-down-cracking is mostly caused by brittle bitumen at low temperatures, and bottom-up-cracking is caused by (high-cycle) fatigue in the base-course and not by large deformations.

Material modelling uses the widely-used generalised Maxwell model. It has the advantage that data from cyclic experiments — which are often conducted in road engineering — can readily be used for parameter estimation. The problem of bad conditioning of the least-squares problem has been tackled using Tikhonov regularisation. The state of the art has been extended regarding geometry modelling. An iterative algorithm has been developed that can generate PSDs using angular and irregular particles. Its flexibility has been proven by the generation of geometries for several different asphalt mix types. Since sieve size is an ambiguous quantity for irregular particles, but a pivotal quantity for PSDs, reliable sieve size estimators have been identified using experimental and synthetic data.

The similarity between the synthetic VT-based data and data from XRCT-scanning has been investigated and found to be satisfactory. Additional investigations have established, that this also holds for particles of the synthetic PSDs. Some shortcomings, which have been revealed after publication of the articles contained in this dissertation have also been addressed and hopefully resolved in a satisfying manner. The major outcome of these investigations is the successful macroscale validation of upscaling methodology.

6.1 Outlook

As always, there is a lot of room for improvement. First of all, the macroscale validation revealed that the success of the macroscale prediction critically depends on mortar design. However, there is no consensus yet about the “true” composition of mortar. Additional experimental investigations are necessary to elucidate the state, in which the mortar actually exists in asphalt.

Particle shape can undoubtedly be improved. Particularly regarding non-convexity of grains. However, it is not known whether it is worth the effort, at least for stiffness predictions.

In contrast to the widely used Discrete Element models of asphalt, the inter-particle contact has not been addressed. How modelling the granular scaffold can be performed in a numerically efficient way in a FE framework remains to be investigated.

The long-term goal of dimensioning pavements based on mesoscale data requires strength and lifetime predictions, which is one of the most challenging tasks in mechanics given a material with the complexity of asphalt.

7 Appendix

The **Abaqus** user manual can lead to a lot of confusion about how to use the generalised Maxwell model correctly. Thus, its usage is documented here. Furthermore, an analysis of required voxel size for accurate reconstruction of shape quantities is conducted.

7.1 Linear Viscoelasticity in Abaqus

Both time domain and frequency domain viscoelasticity require a similar input pattern in **Abaqus**. The material parameters of the generalised Maxwell model have to be converted. In chap. 22.7.1: “Frequency-dependent test data” of the **Abaqus** manual, it is mentioned that the moduli of each Maxwell-chain have to be normalised either with respect to the instantaneous, g_0 , or the long-term modulus, g_∞ , cf. equation 3.3. Furthermore, **Abaqus** requires Prony-series parameters for shear and bulk modulus. Instantaneous, or long-term moduli have to be specified as Young’s moduli. Therefore, the Poisson’s ratio, ν , needs to be known. If the parameters are normalised w.r.t. g_0 , and the computation is carried out in frequency domain, **Abaqus** issues a warning in the *.dat file

```
***WARNING: MODULI=INSTANTANEOUS ON *ELASTIC CANNOT BE USED WITH FREQUENCY  
DOMAIN VISCOELASTICITY. THE MODULI ARE CONVERTED TO LONG TERM  
MODULI USING THE PRONY SERIES PARAMETERS.
```

but continues execution of the *.inp-file. The instantaneous modulus is the sum of all moduli, i.e. the asymptotic high-frequency modulus

$$g_0 = g_\infty + \sum_{i=1}^n g_i . \quad (7.1)$$

It always exists. In contrast, g_∞ vanishes for many materials, which do not exhibit a low-frequency elastic plateau. Whether this is the case can easily be determined from the loss angle, which approaches zero for low frequencies if an equilibrium spring is present. The rest of the material definition stays the same. The Prony-series parameters for **Abaqus** are computed via

$$\bar{g}_i = g_i / g_0 . \quad (7.2)$$

Please note that in the case of $g_\infty = 0$, the sum of the parameters equals unity. In general

$$g_\infty = g_0 \left[1 - \sum_{i=1}^n \bar{g}_i \right] = g_0 - \sum_{i=1}^n g_i, \quad (7.3)$$

holds. Thus, given either g_0 , or g_∞ , the other one can always be computed from the Prony-series parameters. However, if a small equilibrium stiffness is chosen, precision becomes critical. Hence, the parameters have been exported from **Matlab** using **format longEng**. An example of a linear viscoelastic material definition in an **Abaqus *.inp**-file is given below. Please note, that the Poisson's ratio has been set to 0.35 as it has been done in section 2.4 and section 3.3.2. However, this is an estimate. The real Poisson's ratio of bituminous mortar is unknown to the author and furthermore not constant [144; 169; 108; 99].

```
*Material, name=Mortar
*Density
0.0
*Elastic, moduli=instantaneous
2.07217551932997e+003, 0.35
*Viscoelastic, frequency=PRONY
384.148825217030e-003, 0., 20.0877812494278e-006
270.515086959875e-003, 0., 137.313550387470e-006
193.288598923704e-003, 0., 938.630846577418e-006
103.914203049581e-003, 0., 6.41617570633461e-003
36.4443913609555e-003, 0., 43.8588938821572e-003
8.78885060840141e-003, 0., 299.805158182807e-003
2.30327879475844e-003, 0., 2.04937071861688e+000
419.344273517860e-006, 0., 14.0088328292315e+000
154.506977695221e-006, 0., 95.7598327401701e+000
21.6108560541369e-006, 0., 654.583124676234e+000
```

In order to avoid the warning, an artificial equilibrium stiffness can be chosen. In order not to affect the behaviour in the frequency regime of interest negatively, a spring stiffness of $g_\infty = 0.001$ MPa is chosen.

```
*Elastic, moduli=long term
2.70000000000000e-003, 0.35
```

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