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CONSTRUCTION OF STATISTICALLY EQUIVALENT PERIODIC UNIT CELL OF ASPHALT MIXTURE

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Summary: *The paper offers a novel approach to the modeling of asphalt mixtures. It introduces a concept of so called statistically equivalent periodic unit cell (SECUP) known from the analysis of random composites. Such a unit cell allows us to take into account a microstructure of asphalt mixture while keeping the computational cost of the underlying nonlinear analysis relatively low. In particular, the original microstructural configuration is first quantified using a suitable statistical descriptor (two–point probability function). Then a SEPUC is found such that it approximates the target microstructure as close as possible in terms of the selected statistical descriptor. We expect that a sufficiently representative number of 2D micrographs will provide the desired information for constructing even a fully three-dimensional periodic unit cell. At last, the classical first order homogenization technique will be used to extract the effective homogenized properties.*

1. Introduction

The goal of our research is to develop a conceptual approach to the modeling of thermo-mechanical response of asphalt mixtures subjected to external actions. The solution strategy relies on a popular uncoupled multi-scale homogenization technique taking advantage of the concept of statistically equivalent periodic unit cell.

The failure of the particular pavement layers is often caused by the rapid growth of the transit intensity which leads to excessive pavement loading. The pavement design is nowadays based on the empirically gained experiences and on a number of rheological experiments. Up to now there is no material model of asphalt available that would take in account all the influencing aspects of its behavior such as heterogeneity of the material, the nonlinear viscoelastic behavior of bitumen, formation of microcracks, the influence of temperature, fatigue of material etc.

Our topic aims at proposing a material model for the mechanical behavior of asphalt allowing for optimization of the asphalt structure as well as the formation of pavement layers in order to minimize the failure occurrence and to achieve maximal performance of the asphalt pavements.

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2. General approach to modeling of asphalt mixtures

Owing to complicated interaction of geometry, climate, loading and material characteristics that determine the pavement performance it is unrealistic to think that the mechanical response of asphalt mixtures can be captured by a single test. For this reason the authors of paper believe that future developments in the direction of performance based specifications for pavement design should aim at developing a better understanding of asphalt concrete response and the damage mechanism that the material exhibits. To gain such an understanding one needs both sophisticated tests and realistic material models.

Asphalt is a very complex heterogeneous and time-dependent material. In general it is composed of bitumen matrix, aggregates and voids (see Figure 1).

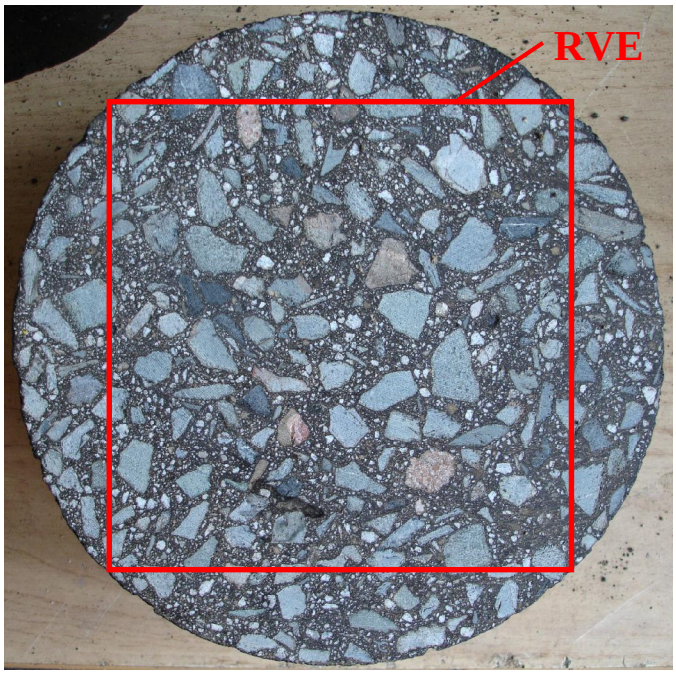


Figure 1 Microstructure of an asphalt mixture, RVE

Bitumen matrices could be divided into four different groups. The first group, still widely used, considers a traditional bitumen matrix without any additives to adjust its behavior. The second group is represented by a bitumen matrix modified by polymeric admixtures, which allows for wider temperature diversity than the traditional bitumen matrices. The next group covers low-viscosity bitumen matrices, which are characterized by a good workability at lower temperatures and yet by keeping their mechanical properties at service temperature. The last group assumes a multi-graded bitumen matrix with temperature diversity extended similarly to the bitumen matrix modified by polymeric admixture. The asphalt mixtures are further divided into compacted and molted. The main difference between the two types of matrices is in the volume fraction of individual phases, in the mixture and in the different processing temperature.

From the material behavior point of view, bitumens are viscoelastic materials and their behavior varies from purely viscous to wholly elastic depending upon loading time and temperature. We expect to treat these properties within unified model capable of describing

the time dependent behavior of all types of asphalt concrete. The model parameters should, nevertheless, be derived from simple experiments.

Up to date tools for the design and analysis in road engineering are based on multi-scale modeling strategies suitable primarily for heterogeneous materials such as asphalt. Homogenization procedures building on the existence of periodic fields usually provide the stepping stone of the analysis.

Apart from constitutive modeling the structural analysis generally requires, due to the above mentioned complex microstructure, analysis on various scales. The computational cost of a fully coupled micro-macro simulation is still, however, relatively high. A significant reduction of the computational cost is fortunately available, particularly if restricting the attention to a fully uncoupled analysis. In this context, response of the representative volume element (RVE) (the sample of a material large enough to reflect statistical fluctuations on the level of observation when subject to a given macroscopic loading path) is of the main interest, see Figure 1. Clearly, such an approach leads to a substantial loss of data when compared with the coupled analysis when individual scales interact with each other and no close-form constitutive relation is needed on the macro-level. If, on the other hand, a macroscopic constitutive law is postulated on the macro-scale, the uncoupled approach allows for providing inputs for the model by a pure simulation without a need for expansive laboratory experiments on complex asphalt structures.

Even the highly simplified fully uncoupled approach depends, however, on an existence of the RVE. The approach essentially relies on the description of microstructure statistics [Zeman – Šejnoha, 2006]. In particular, the original microstructural configuration is first quantified using suitable statistical descriptors (two – point probability function) and then a statistically equivalent periodic unit cell (SEPUC) is found such that it approximates the target microstructure as close as possible in terms of this descriptor.

Following the formulation of SEPUC the attention will turn to the application of well established homogenization technique based on periodic fields [Michel – Moulinec – Suquet, 1999] to derive the effective macroscopic parameters of the composite.

The idea of using totally uncoupled multi-scale procedure stems from the expected possibility of describing the behavior of both the bitumen matrix and homogenized asphalt mixture using the same material model – the generalized nonlinear viscoelastic Leonov model (see [Tervoort, 1996], [Šejnoha – Valenta – Zeman, 2004] extended for the influence of temperature and the value of mean stress. In addition, introducing a damage parameter will allow for the model to keep track of a gradual loss of material integrity when exceeding the tensile strength.

Finally, clearly visible excessive deformation patterns of pavements inevitably call for an implementation of the proposed constitutive model in a large strain setting.

3. Basic statistical descriptors

To reflect a random character of heterogeneous media it is convenient to introduce the concept of an ensemble – the collection of a large number of systems which are different in their microscopical details but identical in their macroscopic details. In the context of quantification of the microstructure morphology, an ensemble represents the collection of

material micrographs taken from different samples of the material. To describe a random microstructure we introduce a *characteristic* function $c_{\mathbf{r}}(\mathbf{x}, a)$, which is equal to one when point **x** lies in the phase r within the sample a and equal to zero otherwise

$$\chi_{\mathbf{r}}(\mathbf{x},\alpha)=\begin{cases}1 & \mathbf{x}\in D_r(\alpha)\\ 0 & \text{otherwise}\end{cases} \tag{1}$$

The symbol $D_r(a)$ denotes here the domain occupied by r-th phase in the sample a. For a two-phase asphalt, $r = s, b$, characteristic functions $c_{\mathbf{s}}(\mathbf{x}, a)$ and $c_{\mathbf{b}}(\mathbf{x}, a)$ are related by

$$\chi_s(\mathbf{x},\alpha)+\chi_b(\mathbf{x},\alpha)=1. \tag{2}$$

With the aid of function $c_{\mathbf{r}}$, the *general n-point probability* function $S_{r1,\ldots,rn}$ is given by [Beran, 1968]

$$S_{r_1,\mathbf{K},r_n}(x_1,\mathbf{K},x_n)=\overline{\chi_{\mathbf{r}1}(\mathbf{x}_1,\alpha),\mathbf{K},\chi_{\mathbf{r}n}(\mathbf{x}_n,\alpha)}. \tag{3}$$

Thus, $S_{r1,\ldots,rn}$ gives the probability of finding n points $\mathbf{x}_1; \ldots; \mathbf{x}_n$ randomly thrown into the media located in the phases $r_1; \ldots; r_n$. We limit our attention to functions of the order of one and two.

Analysis of random composites usually relies on various statistical assumptions such as ergodic hypothesis, spatial homogeneity or isotropy, which may simplify the computational effort to a great extent. In particular, the ergodic hypothesis demands all states available to an ensemble of the systems to be available to every member of the system in the ensemble as well [Beran, 1968]. Then, the *spatial* or *volume average* of function $c_{\mathbf{r}}(\mathbf{x}, a)$ given by

$$\langle\chi_{\mathbf{r}}(\mathbf{x},\alpha)\rangle=\lim_{V\to\infty}\frac{1}{V}\int_V\chi_{\mathbf{r}}(\mathbf{x}+\mathbf{y},\alpha)\,\mathrm{d}\,\mathbf{y}, \tag{4}$$

is independent of a and identical to the ensemble average,

$$\overline{\chi_{\mathbf{r}}(\mathbf{x})}=S_r=\langle\chi_{\mathbf{r}}(\mathbf{x})\rangle=c_r, \tag{5}$$

where c_r is the volume fraction of the r-th phase. Note that the above assumption is usually accepted as a hypothesis subject to experimental verification. The statistical homogeneity assumption means that value of the ensemble average is independent of the position of coordinate system origin. Then, for example, the two-point stone probability function reads

$$S_{ss}(\mathbf{x}_1,\mathbf{x}_2)=S_{ss}(\mathbf{x}_{12}), \tag{6}$$

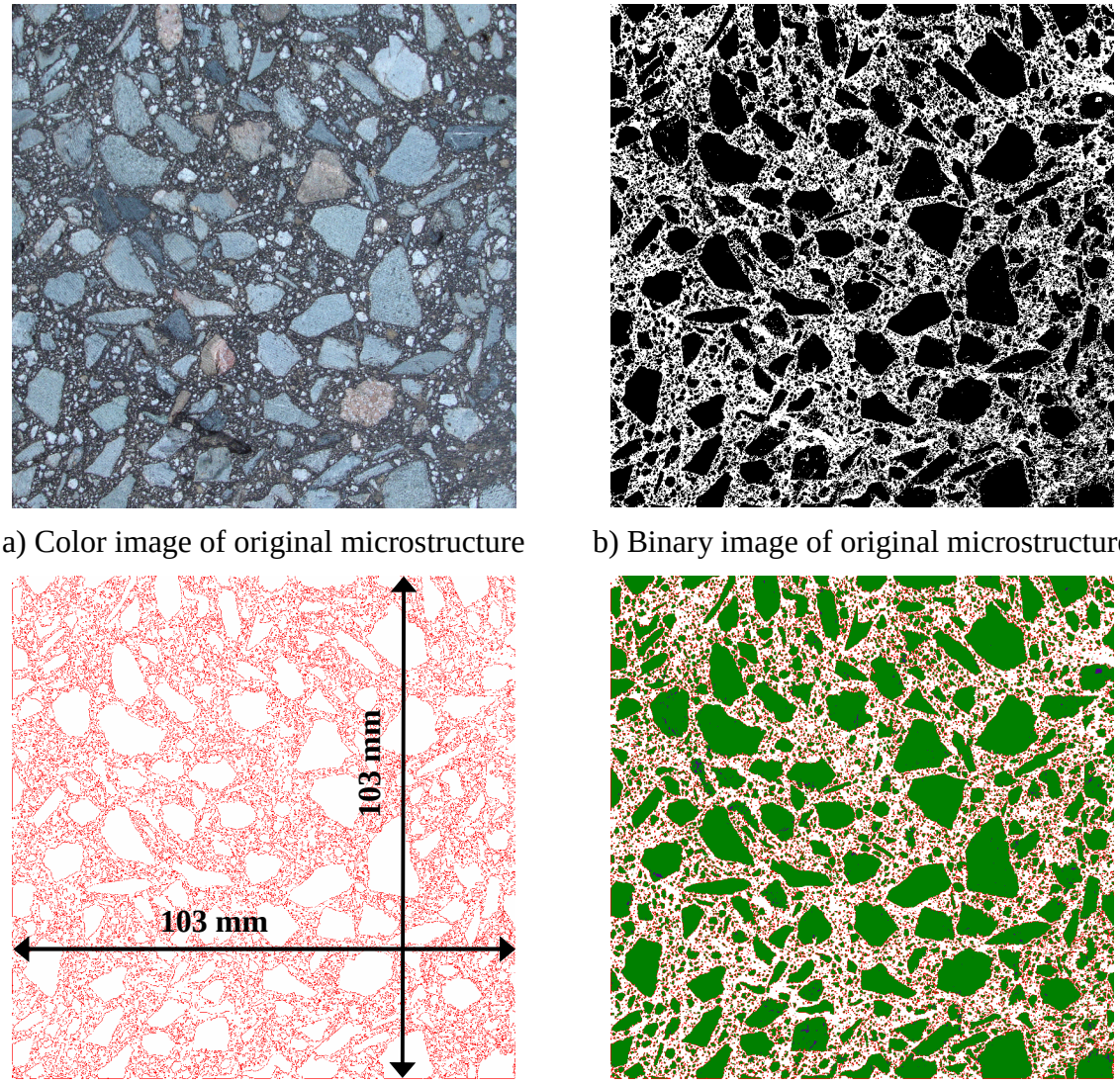
where $\mathbf{x}_{ij} = \mathbf{x}_j - \mathbf{x}_i$. In the context of a representative volume element (RVE: a material element which effectively samples all microstructural configurations) the one-point probability function S_r and the two-point probability function S_{rs} are the same in any RVE (a micrograph of the material sample) irrespective of its position. Thus only one such sample is needed for their evaluation. When constructing the RVE we add an additional requirement with respect to its minimum size. Apart from the above statement we shall require the size of the RVE to be at least such that there exist two points within the RVE which are statistically independent. Then, it appears acceptable to consider a periodicity of the selected RVE. This becomes particularly important when developing an efficient procedure for evaluation of S_r and S_{rs}. Note that for an ergodic and periodic microstructure the two-point probability function S_{rs} receives the following form

$$S_{rs}(\mathbf{x}) = \frac{1}{\Omega}\int_{\Omega} \chi_r(\mathbf{y})\,\chi_s(\mathbf{x}+\mathbf{y})\,\mathrm{d}\,\mathbf{y}\,, \tag{7}$$

where Ω is the size of the RVE (the micrograph area). It is worthwhile to mention that only the Fourier transform of function S_{rs} given by

$$\tilde{S}_{rs}(x) = \frac{1}{\Omega}\,\tilde{\chi}_r(x)\,\overline{\tilde{\chi}_s(x)}, \tag{8}$$

is needed. Note that $\bar{.}$ now stands for the complex conjugate. When introducing a binary image of the actual microstructure may evaluate the last equation very efficiently employing the discrete Fourier transform.



a) Color image of original microstructure

b) Binary image of original microstructure

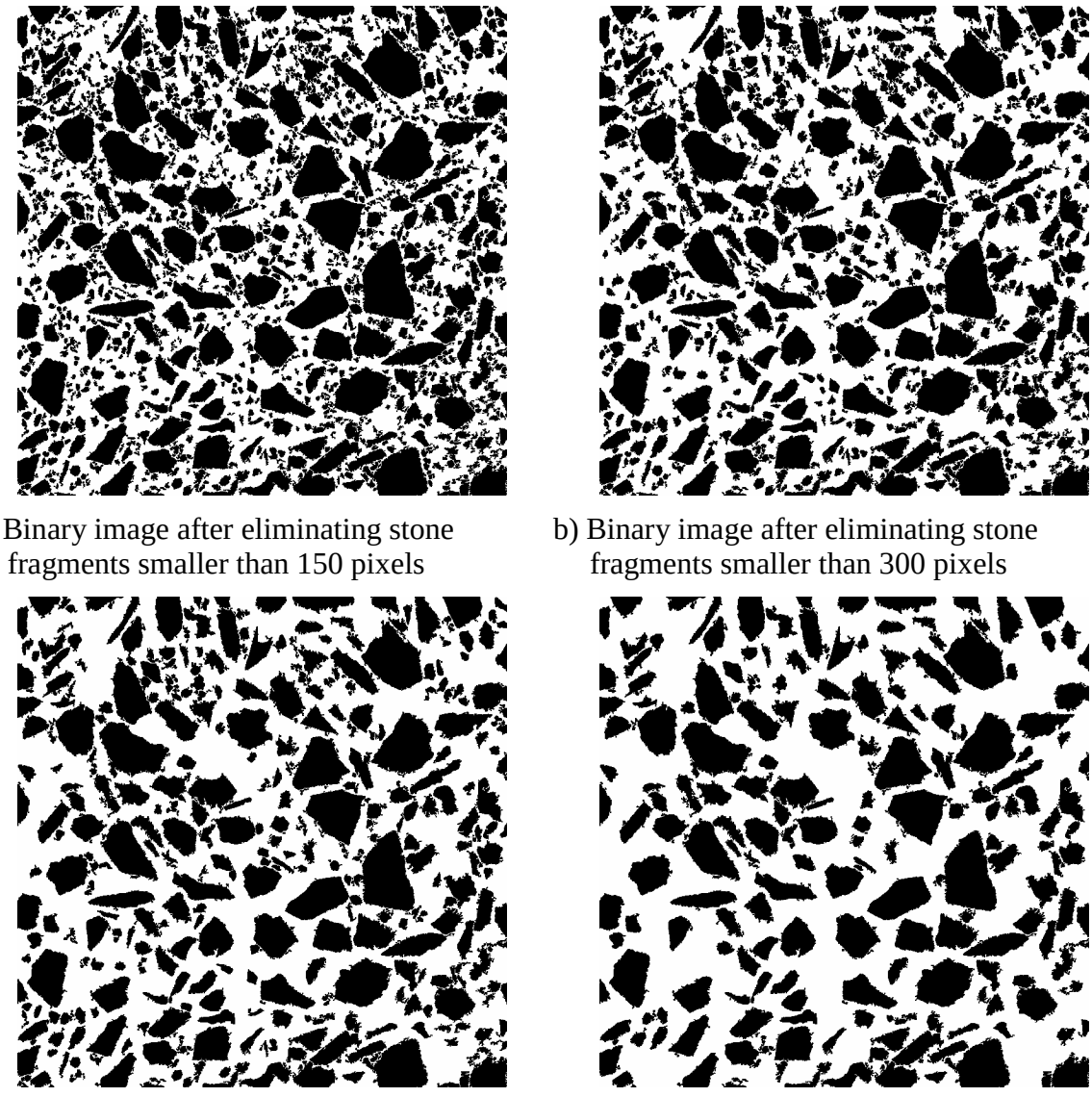
c) Boundary of stones

d) Digitalized bitmap

Figure 2 Bitmap preparation

4. Modification of original sample image

A sample image of real microstructure in Figure 2a was cut out from a large image of asphalt specimen (see Figure 1). The saved image has resolution 1600x1600 pixels. In the first step the real microstructure is replaced by its binary (monochromatic) image. Input color image was modified in freeware graphical software GIMP 2. We created binary image based on tresholding of input color images by means of GIMP program. The tresholding works as setting a range of color scales or intensity and saturation (depends, whether the RGB or HIS representation of image is used), for which the output binary image should be black (or white). A binary version of real microstructure is shown in Figure 2b. Such a digitized micrograph can be imagined as a discretization of the characteristic function $c_s(\mathbf{x}, a)$, usually presented in terms of a $W \times H$ bitmap.



a) Binary image after eliminating stone fragments smaller than 150 pixels

b) Binary image after eliminating stone fragments smaller than 300 pixels

c) Binary image after eliminating stone fragments smaller than 600 pixels

d) Binary image after eliminating stone fragments smaller than 1200 pixels

Figure 3 Examples of binary images of original microstructure

A sophisticated computational tool for the elimination of small stone fragments that are expected to have negligible effect on the homogenized material parameters was developed. This routine determines the boundary of each stone (Figure 2c) and the area in pixels of all stone fragments. The resulting digitalized smoothed bitmap of the original color image is depicted in Figure 2d, where local defects within individual stone fragments were filled and the stones were separated from each other as much as possible. Several examples of the modified original image after eliminating a respective number of stones depending on their size appear in Figure 3.

These images can be related to the Cumulative distribution function of the number of stones linked to a given area plotted in Figures 4 and 5. While Figure 4 shows the entire spectrum, Figure 5 displays only a zoom into a smaller area. Figure 5 in particular suggests the presence of large fraction (from their number point of view) of small stones. From their volume fraction point of view this huge amount of small stones is, however, negligible. This is evident both from Figure 6 and even more from Figure 7.

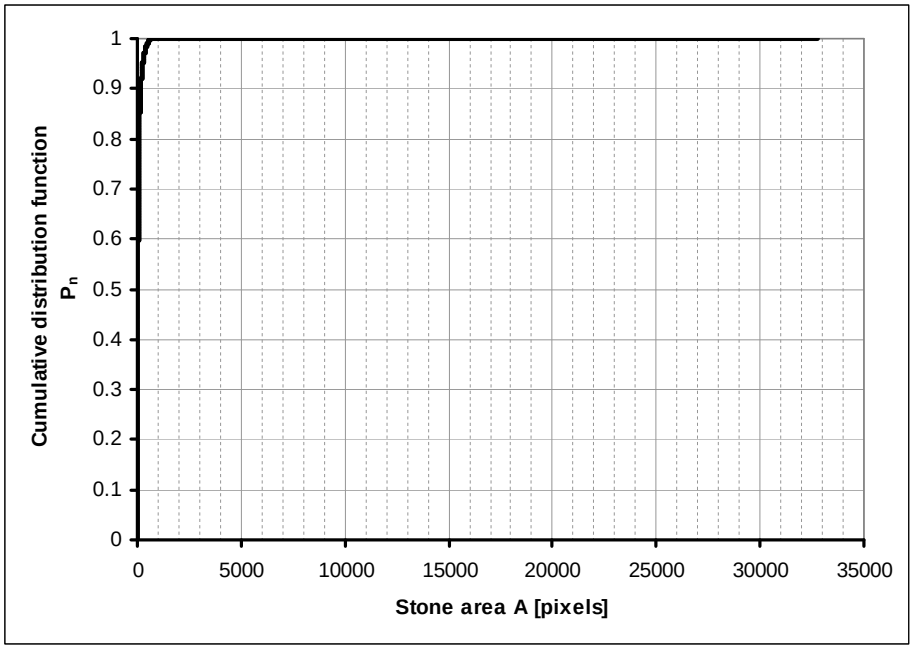


Figure 4 Cumulative distribution function

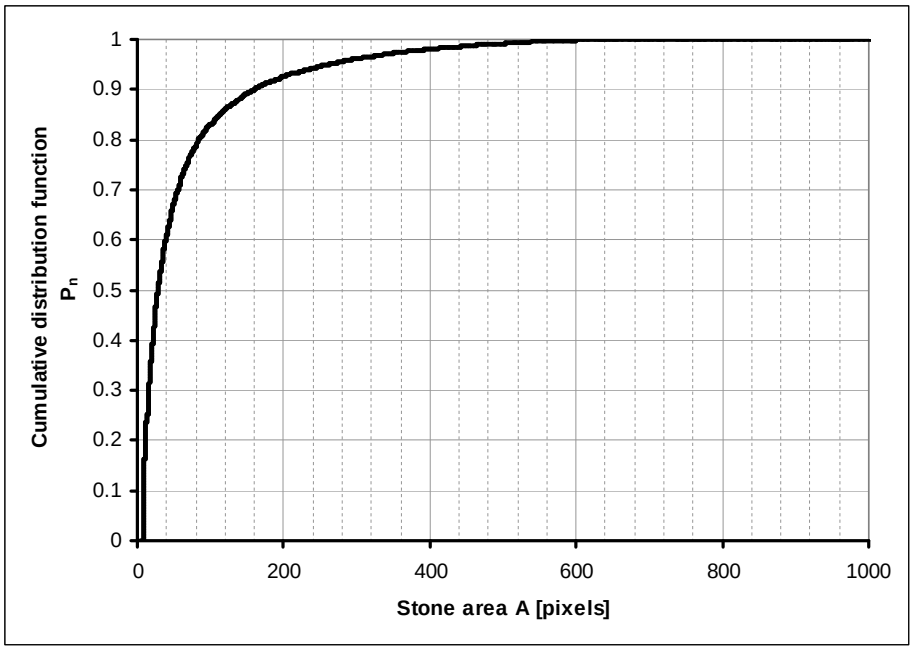


Figure 5 Cumulative distribution function – detail

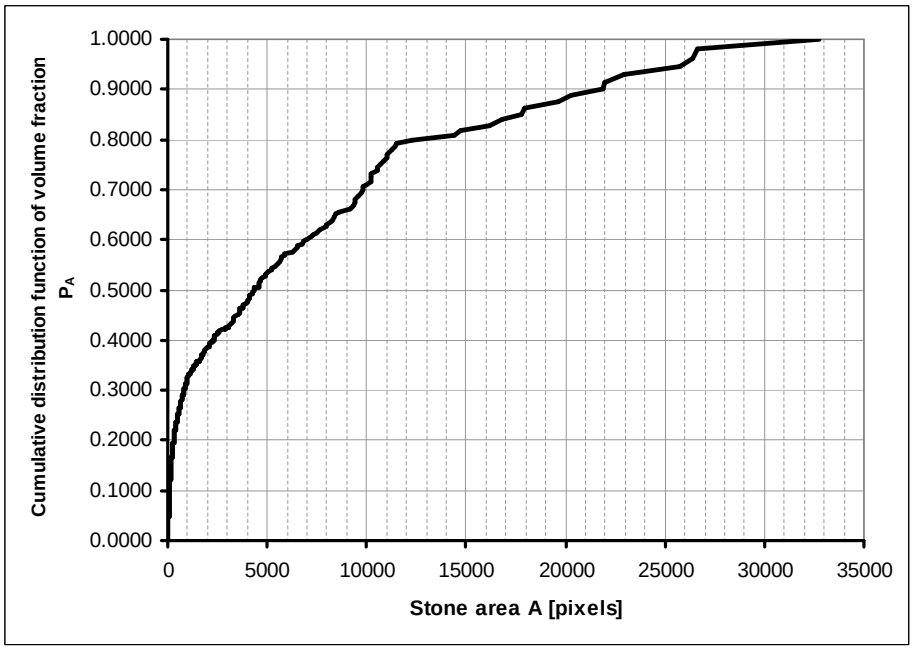


Figure 6 Cumulative distribution function of volume fraction

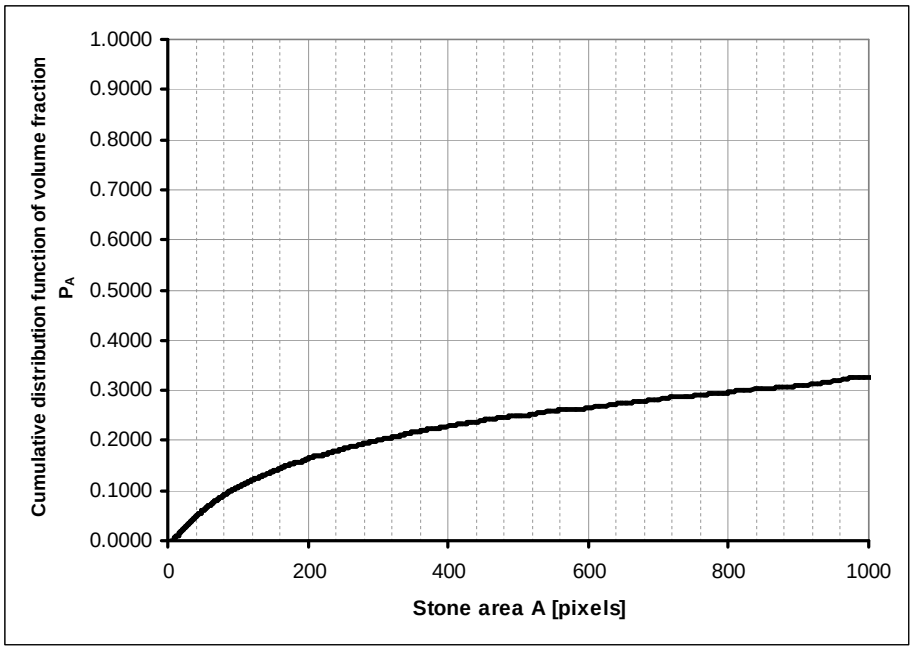


Figure 7 Cumulative distribution function of volume fraction - detail

5. Evaluation of two-point probability function

In preparation for the search for the desired statistically equivalent periodic unit cell it is necessary to evaluate the variation of the two-point probability function, which will serve as a measure of similarity of real microstructure (Figure 3) and a respective periodic unit cell.

With reference to [Šejnoha – Valenta – Zeman, 2004] the two-point probability function is evaluated with the help of Fast Fourier Transform applying directly to a selected binary image plotted in Figure 3. The resulting function for stones under assumption of statistical homogeneity Eq. (7) and (8) appears in Figure 8.

Providing we accept this function to be invariant with respect to rotation we may replace the statistically homogeneous function by its isotropic format derived by averaging the original function in Figure 8 through all possible angles. The corresponding results obtained for individual micrographs in Figure 3 are displayed in Figure 9. These functions in particular are scaled with respect to the corresponding volume fraction; recall Eq. (6) giving its value equal to one if the relative distance of two points is reduced to zero. On the other hand, when the two points are spread far apart the event of throwing simultaneously two points randomly into a medium becomes equivalent to throwing the two points into the medium independently, i.e. $S_{ss}(\mathbf{x}) \rightarrow c_s^2$. Therefore, the sample size should be sufficiently large to comply with this property. This requirement was certainly fulfilled for the present sample. As also evident from the curves in Figure 9, the probability of finding two points both in stones is reduced for the same distance due to removal of stones from the original microstructure. Just the opposite is true for the bitumen phase.

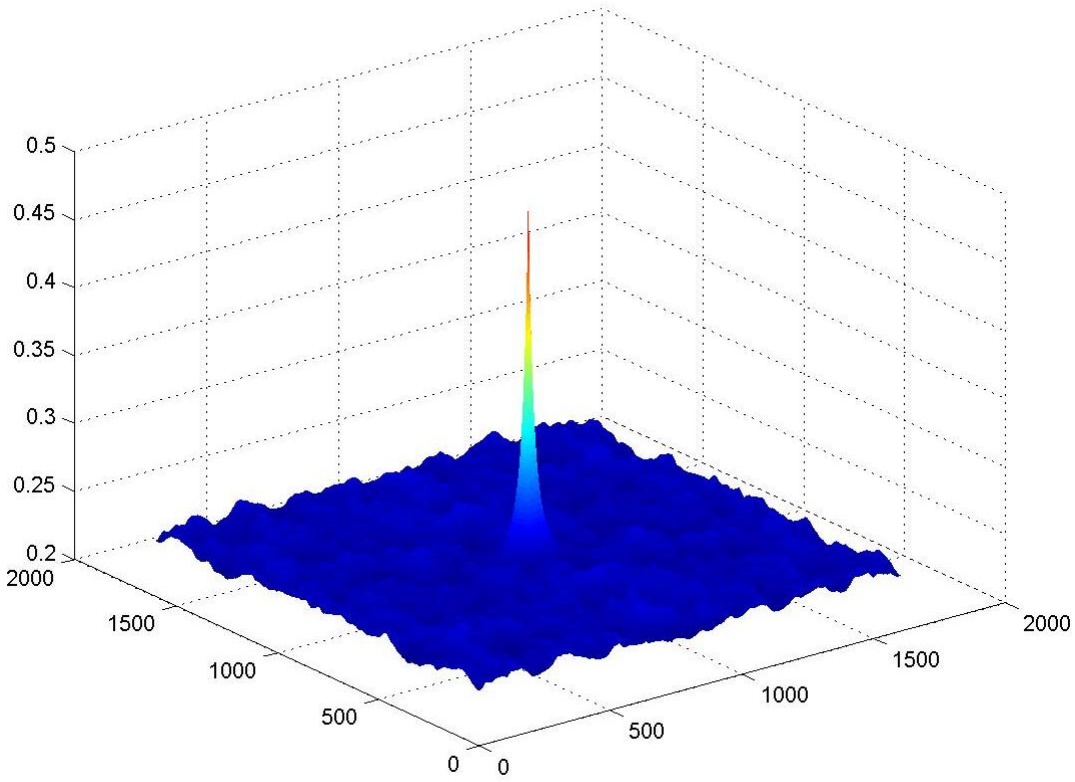


Figure 8 Two-point probability function for binary image A_{elim} = 300px

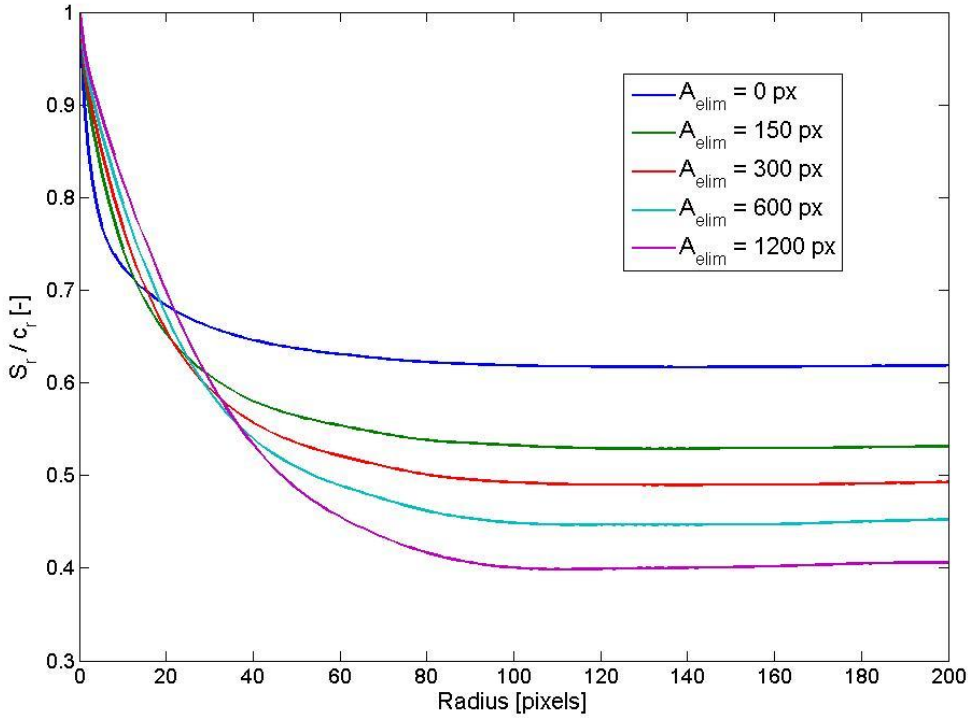


Figure 9 Average two-point probability functions normalized by stone volume fraction c_r

6. Conclusion and future work

This paper presents a summary of the preliminary work on asphalt mixtures. It concentrates on morphological description of actual microstructure. To that end, the two-point probability function is used to provide information about material statistics. The effect of elimination of stones with relatively small size is studied. While the total number of stones eliminated is relatively high their volume fraction when compared to the total volume of stones is negligible. Nevertheless, the effect of elimination becomes pronounced when considering the two-point probability function as shown in Figure 9. Since this function is assumed to govern the search for an equivalent periodic unit cell, it can be expected that keeping the original microstructure intact will be important, particularly from the effective properties point of view. This, however, is the subject of present research and must be yet confirmed.

7. Acknowledgment

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8. References

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