This is an electronic reprint of the original article.
This reprint may differ from the original in pagination and typographic detail.

Castillo, Daniel; Al-Qadi, Imad

Mechanical Modelling of Asphalt Concrete Using Grid Division

Published in:
INTERNATIONAL JOURNAL OF PAVEMENT ENGINEERING

DOI:
[10.1080/10298436.2019.1650926](https://doi.org/10.1080/10298436.2019.1650926)

Published: 02/07/2020

Document Version
Peer reviewed version

Please cite the original version:
Castillo, D., & Al-Qadi, I. (2020). Mechanical Modelling of Asphalt Concrete Using Grid Division. *INTERNATIONAL JOURNAL OF PAVEMENT ENGINEERING*, 21(8), 1012-1023.
<https://doi.org/10.1080/10298436.2019.1650926>

This material is protected by copyright and other intellectual property rights, and duplication or sale of all or part of any of the repository collections is not permitted, except that material may be duplicated by you for your research use or educational purposes in electronic or print form. You must obtain permission for any other use. Electronic or print copies may not be offered, whether for sale or otherwise to anyone who is not an authorised user.

Mechanical Modelling of Asphalt Concrete Using Grid Division

Journal:	<i>International Journal of Pavement Engineering</i>
Manuscript ID	Draft
Manuscript Type:	Original Article
Keywords:	multiphase material, modelling, grid division, finite elements, microstructure

SCHOLARONE™
Manuscripts

1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32
33
34
35
36
37
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59
60

MECHANICAL MODELLING OF ASPHALT CONCRETE USING GRID DIVISION

Abstract: In this paper, a simple method is introduced for the computational modelling of multiphase materials, and for the approximation of their mechanical response. The two-dimensional microstructures of six asphalt concrete specimens are selected; three of the specimens have ‘low’-, and three have ‘high’ aggregate fraction. A grid is used to divide the surface of each microstructure into square cells. The procedure of grid division is applied from 1 up to 100 divisions per side (i.e., up to 10,000 cells in the grid-divided specimen). To obtain an approximation of the mechanical response of the microstructure, the properties of the cells are estimated using three simple interpolation rules between the properties of the two phases, i.e. asphalt matrix and rock aggregates. It is found that the interpolation rules can yield reasonably representative results depending on the aggregate fraction of the microstructures and the number of divisions/cells in the grid. The grid-divided specimens allow approximating the overall mechanical response of the microstructures, and characteristics such as strain concentrations, overall deformations, and resulting force.

Keywords: multiphase material, modelling, grid division, finite elements.

1. INTRODUCTION

The process of modelling multiphase materials in two and three dimensions can become quite complex, depending on the accuracy desired in the geometric and mechanical description of the individual phases. Commonly, a modeling process requires laboratory resource-and computational cost-intensive efforts. This process may entail acquiring the geometry of multiple phases composing the material, i.e. through imaging or X-ray analysis of cored specimens (Masad et al. 1999, Gruber et al. 2012, Obaidat et al. 2017), as well as laboratory testing of individual phases to quantify their associated mechanical or physical characteristics of interest, such as moisture/thermal diffusivity, stiffness, surface free energy or linear viscoelastic parameters (Kim et al. 2005, Kim et al. 2008, Yokohama and Nakashima, 2005, Witthüser et al. 2006). The process may also involve the formulation or usage of heavy, time-consuming computational models, that need calibration to yield representative results. Understandably, such a process necessitates a trade-off between result accuracy and computational costs. Hence, alternatives to de-escalate the complexity of the modelling process should be considered, geared towards time- and cost-efficient models that consume fewer resources.

In this context, there is interest in the area of pavements to adequately characterize the geometry and mechanical behavior of the multi-phase materials that compose the pavement structures, as well as numerous variables that simultaneously affect their properties, such as temperature, moisture, stress regime and oxidation. To this end, complex models have been developed by several researchers to represent pavement materials and structures. Many of these models use the finite element (FE) method and focus particularly on the behavior of asphalt concrete (AC) mixtures. Such models have been developed to predict damage and visco-plastic behavior of material under loading (Darabi et al. 2011), aging (Rahmani et al. 2017), and fracture using the cohesive-zone theory (Aragão et al. 2010). Tire-pavement interaction has

also been considered, using measured three-dimensional contact stresses (Wang and Al-Qadi, 2009), including various tire configurations such as wide-base tires, and considering non-linear anisotropy in the lower layers of the pavement structure (Hernandez et al., 2016). In addition, the impact of uncertainty and variability on AC behavior has been studied, through random correlated spatial variability and the random generation of micromechanical configurations, as well as the usage of domain analysis methods to quantify 'bulk' damage potential (Castillo and Al-Qadi, 2018; Caro et al., 2018; Gamez et al. 2018).

These models take advantage of the versatility of the FE method to provide a representative spatial discretization of the domain of interest, and to accurately consider appropriate constitutive behaviors of the composing phases of the materials or the layers of the structure. The computational models are based on previous validations of FE predictions and provide good matches with experimental results; for instance, using viscoelastic approximations for the behavior of the AC material has proved useful for modeling distresses, such as rutting (Elseifi et al. 2006). This constitutive model was also used to predict strains in full-depth flexible pavement sections under moving loads (Wang and Al-Qadi, 2008).

In the context of the FE model, the domain of interest (i.e. the multi-phase geometry) commonly needs a finer discretization around irregularities in the material, near which critical concentrations of stresses and strains are expected to develop. Moreover, the need to consider thousands of irregularly-shape aggregates and air voids is a shortcoming. The presence of these numerous irregularities and inclusions is responsible for a significant part of the computational cost of the modeling process; characteristics such as the low thickness of the asphalt matrix between highly angular aggregates, or a high density of air voids over a small area, are directly responsible for inducing finer-than-average meshes. Considering these characteristics results not only in a greater number of finite elements, but it also hinders the meshing process and may result in non-suitable element shapes that compromise the results (i.e. leading to ill-conditioned

matrices in the FE model). Moreover, the modelling of pre-existing cracks within the material, as well as additional parameters inherent to the model such as interaction laws between the phases, add to the complexity and associated computational cost of the models.

An alternative that has been used to address these challenges is multiscale modeling. A multiscale model alternates between a local, heterogeneous representation of the microstructure of the material, and a global, statistically homogeneous model of a structure. The scales are coupled two-way and linked through homogenization; multiscale models can include nonlinear behavior and fracture, and significantly reduce computational times using parallelization techniques (Kim et al. 2013). The local representation should be large enough to be representative of the global behavior of the mixture, but still small enough to be computationally efficient. This smallest practical unit is called a representative volume element (RVE); for instance, an RVE of 60 mm was found for a Superpave mixture with 12.5 mm nominal maximum aggregate size (NMAS) using digital image correlation (Kim et al. 2010), and in general, statistical homogeneity in the fraction of inclusions is observed from sizes greater than 2-3 times the NMAS, at least in two dimensions (Ozer et al. 2016). Multiscale experimental data shows different levels of sensitivity depending on the scale (Underwood and Kim, 2013), through temperature and frequency sweep tests at the scales of binder/mastic, fine aggregate matrix, and asphalt mixtures.

While the approach presented herein is not multiscale, it certainly shares many of the basic characteristics of multiscale modeling. These include discretizing phases at different scales, the search for a scale/size that is representative of the actual overall response, homogenizing mechanical/physical properties of the material, and in general, offering a computationally efficient alternative to model phenomena over a highly heterogeneous domain. The main difference between the two approaches is the presence of a *range* of scales (multiscale modeling uses ‘leaps’ between scales, whereas in the presented approach the range is

1
2
3 94 continuous), and therefore the lack of feedback between scales.
4

5 95 This paper offers an intermediate approach, half-way between micromechanics and
6
7
8 96 continuum-damage based modeling, to approximate the response of two-dimensional
9
10 97 specimens of AC. By discretizing their phases (aggregates and matrix) and estimating
11
12 98 mechanical properties over a grid, the complexity of the model is reduced without neglecting
13
14 99 the presence and effects of irregularities and inclusions in the domain.
15
16

17 100

18
19 101 **2. METHODOLOGY**

20
21 102 The present study follows four steps to obtain a range of estimates of the response of asphalt
22
23 103 concrete (AC) microstructure:
24

- 25
26 104 - *Step 1:* Superimpose a grid on the surface of the microstructure, to divide it into cells.
27
28 105 - *Step 2:* Determine the aggregate fraction per cell, i.e. the percentage area of the cell that is
29
30 106 covered by the aggregate phase.
31
32 107 - *Step 3:* Estimate the mechanical properties cell-wise, interpolating between the properties
33
34 108 of cells with 0-100% aggregate fraction.
35
36 109 - *Step 4:* Create an FE model of the grid-divided specimen in axial compression.
37
38
39

40 110 Three alternatives are tested to estimate the mechanical properties of the cells in Step 3 (see
41
42 111 Section 2.3), which involve simple interpolation rules between the properties of the two ‘pure’
43
44 112 phases; rock aggregates and matrix. Herein, the aggregate fraction was selected as the
45
46 113 determining parameter of mechanical behavior, since the (instantaneous) stiffness of the coarse
47
48 114 aggregates can be two or three orders of magnitude greater than that of the binder. The steps
49
50 115 are described next.
51
52

53 116

54
55
56 117 **2.1. Division of the microstructure into cells, using a grid (Step 1)**

57
58 118 *2.1.1. Selection and mechanical properties of the AC specimens*
59
60

1
2
3 119 The objective of the first step is to partition the surface of the specimen into cells. A 'specimen'
4
5 120 is understood as a microstructure of AC, i.e. a two-dimensional configuration of aggregate
6
7 121 particles embedded in a homogeneous matrix of fine aggregates, asphalt binder and air. For
8
9 122 simplicity, in this study the specimens are composed of two phases only, namely coarse
10
11 123 aggregates and asphalt matrix. For simplicity, in this application the phases are not susceptible
12
13 124 to damage, i.e. there is no reduction in the ability to sustain stresses.
14
15

16
17 125 Two values of aggregate fraction are considered in this study: a 'low' aggregate fraction of
18
19 126 52.7%, and a 'high' aggregate fraction of 66.1%. The values of aggregate fraction tend to vary
20
21 127 over a relatively wide range. The selected values are within the range of two sources (You *et*
22
23 128 *al.*, 2009, Zelelew and Papagiannakis, 2011). For each aggregate fraction, three AC
24
25 129 microstructures were randomly generated, for a total of six microstructures of AC. Two values
26
27 130 of aggregate fraction are used because the aggregate phase is expected to have a major
28
29 131 influence in the mechanical response of the microstructures, due to the high stiffness of the
30
31 132 rocks. The microstructures are squares with 100-mm sides; the shape and size were arbitrarily
32
33 133 selected, to be within the scale of laboratory specimens. The microstructures are presented in
34
35
36
37 134 Figure 1.
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59
60

Figure 1. AC microstructures selected for the grid division and modelling approximation. (a) Low aggregate fraction, 52.7%. (b) Higher aggregate fraction, 66.1%.

The AC microstructures were created randomly, using a MATLAB code first presented by Castillo *et al.* (2015) and now in its latest version (MG, microstructure generator). In this study, a microstructure is understood as a random spatial configuration of polygons with aggregate-like characteristics, which are placed within a domain with arbitrary shape. Prescribed criteria can be followed, such as probabilistic rotation and/or location of the particles. The microstructures are created in two dimensions, using an algorithm to create the shapes of the aggregates (i.e. without using an aggregate database). Criteria used include a random number of vertices for the aggregates, random distances from each vertex to the center of the aggregate,

and random elongation. The MG is capable of achieving various levels of aggregate angularity and microstructure forms (Castillo *et al.* 2015).

The objective of having three microstructures for each aggregate fraction (i.e., replicates) is to assess the consistency of the results; in other words, to observe if the behavior presented by any of the specimens is representative of their corresponding aggregate fraction. A key for this assessment is consistency among microstructures, i.e. gradation of the particles is the same for all microstructures, and the two levels of aggregate fraction are kept almost constant among specimens. Herein, consistency was achieved by the procedure of random generation of the microstructures provided by the MG. The aggregate size of the microstructures presented in Figure 1 ranges from 1.18 mm (sieve #16) to 19 mm (sieve 3/4’’).

2.1.2. Grid pattern

Figure 2 presents three possible ‘tiling patterns,’ or ways to divide a two-dimensional domain using a grid of cells with the same size and/or shape; squares, equilateral triangles, and regular hexagons. As observed, there are many ways of dividing a domain into cells; consider that the cells could also be combined to create arrays of cells of the same shape and different size.

Figure 2. Three possible ways to divide a plane using a regular grid. (a) Square cells, (b) Triangular cells, (c) Hexagonal cells.

1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32
33
34
35
36
37
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59
60

Although any tiling pattern could be used to divide the specimens, in this study the microstructures are divided into square cells of equal size, which is perhaps the simplest way to divide a plane and the most computationally favorable. Using this pattern, the grid resolution can easily be doubled, which simplifies increasing the divisions (i.e. the ‘next’ grid with more divisions is relatively easy to produce). Also, all even- and odd- divided specimens will always have some nodes in the same position.

2.2. Cell-wise determination of the aggregate fraction (Step 2)

The six microstructures were divided using grids, in the (full) range from 1 to 100 divisions, i.e. partitioning them into 1 to 10,000 cells. Selected divisions corresponding to microstructures L1 and H1 from Figure 1 are presented in Figure 3.

Figure 3. Grid division and aggregate fraction of (a) microstructure with low aggregate fraction ('L1' from Figure 1), and (b) microstructure with high aggregate fraction ('H1' from Figure 1). The colors represent the percentage area of each cell that is covered with aggregates.

1
2
3 183 Notice that quite early in the division process, some cells are already covered completely by
4
5 184 aggregates, and for higher numbers of divisions (or microstructures with low aggregate
6
7 185 fraction) there are also cells that comprise only asphalt matrix. These cells may prove critical
8
9 186 to the overall response of the specimen, since they will perform purely as aggregates or matrix,
10
11 187 without any kind of interpolation.
12
13

14
15 188 The grid-divided specimens from Figure 3 can be interpreted as representations of the
16
17 189 microstructures at different 'resolutions' (scales), ranging from very coarse (low resolution,
18
19 190 less than 10-20 divisions of a 100-mm side) to detailed (about 30-40 divisions and upwards,
20
21 191 for the scale used in this study). The maximum number of divisions in the grid (100) was
22
23 192 selected arbitrarily; as the number of divisions increases, the original aggregate microstructure
24
25 193 becomes more discernible.
26
27

28
29 194 Because of the complex geometry of the aggregates, calculating the aggregate fraction per
30
31 195 cell can be challenging. The uniform grid frequently isolates highly irregular partitions of
32
33 196 aggregates and matrix, and these areas become difficult to account for. Additionally, the
34
35 197 increased number of cells is a challenge, even for a specimen with relatively low divisions. In
36
37 198 this study, an automated meshing procedure was devised using (1) custom Python scripts and
38
39 199 (2) the built-in meshing algorithm from the general-purpose FE software Abaqus, as follows.
40
41 200 The matrix phase of the specimens was first isolated and partitioned using the grids, and the
42
43 201 resulting (partitioned) matrix phase was meshed with finite elements. The presence of the
44
45 202 partitions guaranteed that (1) no finite element belonged to more than one cell, and (2) the full
46
47 203 domain of the matrix phase was covered with elements. The area of the elements within each
48
49 204 cell was then accumulated (matrix area per cell), and the aggregate area per cell was obtained
50
51 205 by subtraction.
52
53
54
55
56
57
58
59
60

2.3. Interpolation rules to estimate the mechanical properties of the cells (Step 3)

The data resulting from the grid division (Step 2) was used as part of a simplified methodology to approximate the behavior of the microstructures. Considering that the aggregate fraction per cell is known for all (600) grid-divided specimens, an estimate of the mechanical properties of the cells was calculated based on the elastic and linear viscoelastic properties of the ‘pure’ aggregate and matrix phases, respectively, following three interpolation rules.

The aggregate phase was considered to be fully elastic, with a Young’s modulus of 25 GPa and a Poisson’s ratio of 0.16. These values are within the ranges reported for limestone (Shakiba et al. 2015, Yasar et al. 2004, Hart and Wang, 1995). On the other hand, the matrix phase was considered linear viscoelastic, with instantaneous relaxation modulus (E_o) equal to 112 MPa at 25 °C, Poisson’s ratio 0.40, and Prony parameters reported by Kim et al. (2005). The parameters are presented in Table 1. The same set of relaxation parameters is applied to all viscoelastic cells of material, in normalized form.

Table 1. Viscoelastic mechanical parameters of the asphalt matrix, from Kim *et al.* (2005).

E_1 [kPa]	73,173	η_1 [kPa·s]	115
E_2	25,506	η_2	418
E_3	10,847	η_3	1,079
E_4	2,078	η_4	1,529
E_5	332	η_5	2,249
E_6	53.4	η_6	3,513
E_7	8.44	η_7	5,430
E_8	1.33	η_8	8,664
E_9	0.252	η_9	20,406
E_∞	0.122		
ν	0.40		

In any of the three interpolation rules, a cell with 100% aggregate fraction will behave as a

homogeneous block of rock (elastic). Conversely, a cell with 0% aggregate fraction is modelled as a block of matrix (linear viscoelastic). For all other cells with aggregate fractions in the 0-100% range, three simple interpolation rules between the two phases are tested. An example showcasing the three alternatives is presented in Figure 4 for a grid-divided specimen with 40 divisions, i.e. 1,600 cells (microstructure ‘L2’ in Figure 1).

Figure 4. Three simple interpolation rules to estimate the mechanical properties of the cells.

2.3.1. Rule 1. '50/50'

In the first interpolation rule, the mechanical response of a cell is decided using a simple true/false criterion (only two possible outcomes); if the aggregate fraction of the cell is less than 50%, it will behave as pure matrix; on the contrary, if it is over 50%, it will be modelled as pure aggregate. In this way, a cell with 25% aggregate fraction would behave as pure matrix (viscoelastic, instantaneous modulus $E_o = 112$ MPa), and a cell with 75% aggregate fraction

would behave as pure aggregate (elastic, modulus $E = 25,000$ MPa). This interpolation rule is considered to be the simplest approximation to the actual response of the microstructure.

2.3.2. Rule 2. Linear interpolation

A linear interpolation was proposed as the logical step following the aforementioned alternative. In this rule, if the aggregate fraction is not 100%, the cell is modelled linear viscoelastic and its value of instantaneous modulus E_o is found by linear interpolation between the E_o of the matrix and the Young's modulus of the aggregates, i.e., an intermediate modulus between matrix and aggregates, proportional to the aggregate content of the cell. Only if the aggregate fraction is equal to 100% would the cell be modelled as pure rock. For instance, a couple of cells with aggregate fraction 25% and 75% would be modelled linear viscoelastic, with instantaneous modulus E_o 6,300 MPa and 18,800 MPa, respectively.

It can probably be foreseen that the grids with few divisions will result in grossly non-representative responses; however, calculating them is of interest since their results will allow assessing whether the alternatives produce more refined results with increasing divisions, if applicable.

2.3.3. Rule 3. Exponential interpolation

Finally, an exponential interpolation was proposed as a slightly more refined, yet still extremely simplified approximation to estimating the properties of the cells. The idea of testing an exponential interpolation comes, once again, from the difference in magnitude between aggregates and matrix. From the linear interpolation, it may be noticed that there could be an overestimation of the contribution of the aggregates, since it is more likely that the controlling behavior is viscoelastic (due to the matrix), even at relatively large aggregate fractions. To counteract this effect, the exponential interpolation assigns a lighter 'weight' to the influence

of the aggregates when compared to the linear alternative.

A curve of the following shape was used (moduli in MPa):

$$E_o^{cell} = E_o^{matrix} e^{k*AGF} \tag{1}$$

where the instantaneous modulus of a cell (E_o^{cell}) is a function of the modulus of the matrix phase (E_o^{matrix}), the aggregate fraction of the cell (AGF , ranging from 0 to 1) and a constant k that ensures the fit, i.e. if the aggregate fraction is 100% then E_o^{cell} equals the modulus of the rock. For the moduli used in this study, k was equal to 5.4081. Using the exponential interpolation, for instance, a cell with 25% aggregate fraction would behave viscoelastic with an instantaneous modulus E_o equal to 433 MPa (instead of more than 6,000 MPa in the linear interpolation), and a cell with 75% aggregate area will have E_o equal to 6,468 MPa (instead of 18,800 MPa, linear). If the cell is 100% aggregate, it will be modelled as pure rock.

2.4. Conditions for the finite element simulations

As presented in the above sections, six AC microstructures (Figure 1) will be divided using a grid from 1 to 100 divisions, to create 100 grid-divided specimens per microstructure. Also, there are three interpolation rules per grid-divided specimen, which gives a total of 1,800 simulations. Six additional simulations are carried out for the microstructures with no grid-like divisions (i.e. traditional meshing of the microstructures in Figure 1), to provide a comparison and contrast with the results of the grid-divided specimens.

The specimens were modelled in FE under a fixed loading scheme. A total displacement of 0.1 mm in monotonic compression was applied during 0.5 sec on a rigid plate tied to the top of the specimens. In the simulations, the vertical movement at the base of the specimens was restricted, and the plate that applied the displacement moved downwards along the vertical axis only, with no rotation.

A uniform target mesh size of 0.5 mm was selected for both the grid-divided specimens and

the six 'original', undivided microstructures. The grid-divided specimens were meshed with rectangular elements (about 40,000), and the microstructures were meshed with triangular elements (around 90,000). Nevertheless, consider that the meshing of the grid-divided specimens is completely neat, since there are no inclusions or irregularities in the geometry (i.e., square elements meshing square subdivisions on a square specimen). Therefore, a model as 'simple' as those presented in Figure 3 could easily be meshed with only a handful FE, greatly reducing its computational cost.

3. RESULTS AND ANALYSIS

The analysis of results is presented in three stages. First, the strain in the deformed specimens provides an overview of the differences between the three alternatives. Then, a more detailed analysis of the force-displacement curves gives insight into the accuracy associated with each of the alternatives. Finally, a summary of the force at the end of all the simulations is presented.

3.1. Strain in the deformed specimens

Figure 5 presents a selection of grid-divided specimens for one microstructure of AC ('L1' from Figure 1) following the three interpolation rules between the mechanical properties of the matrix and the aggregates. The deformations are plotted with a factor of 30. The grid divisions in Figure 5 correspond to those presented in Figure 3, from 10 divisions upwards.

A clear contrast is observed between the alternatives in the specimens with fewer grid divisions (~20 or less). In rule 1 ('50/50') there is a marked difference between the stiff, elastic blocks of rock, and the blocks of matrix, which are very soft and viscous in comparison. The specimens with linear and exponential interpolation exhibit the presence of the aggregates as well, but their overall behavior is more uniform, and the deformations of the vertical (free) edges of the specimens are smaller than in the first alternative.

Figure 5. Maximum principal strain for selected grid-divided specimens, three interpolation rules. The corresponding microstructure is 'L1' from Figure 1. Notice the difference in the scale among alternatives; results of the full microstructure are identical and differ only in the color scale.

When the number of divisions starts to increase, the behavior of the grid-divided specimens becomes more consistent, and similar traits appear among alternatives. The shapes of the aggregates begin to emerge, and strain concentrations gradually converge to similar values; for example, in the three alternatives the strain on the 'paths' between aggregates already has values that are comparable to the microstructural results (lower part of Figure 5 – there is only one microstructure, presented with three color scales for comparison within the alternatives) as early as 30 divisions. In general, by 50-100 subdivisions the actual shapes of the aggregates, the 'paths' of high strain in the matrix and the strain concentrations from the original microstructure are observable in the grid-divided specimens. The improvement in the representation of certain characteristics of the actual behavior is a consequence of the increase in 'resolution,' i.e. the accuracy of the geometric representation of the aggregates.

When comparing the results from the grid-divided specimens with the response of the associated microstructure, the three alternatives seem to be converging towards the microstructural response with an increasing number of grid divisions. The convergence is happening at different rates, however; the exponential interpolation appears to offer a closest match with the microstructure 'earlier' (at a lower number of divisions) than the other two alternatives.

The methodology used herein produces simplified models in terms of computational cost. Given the conditions in this study, grid-divided specimens were two-dimensional and had less than 50,000 elements. It was possible to (a) create, (b) run and (c) analyze (extract data) from a considerable number of simulations in bulk (1,800), in an estimated cumulative time of 3-4 days, using a common office computer. Hence, the development of one simulation would take approximately 3 minutes to run, from start to finish. In contrast, three-dimensional full microstructural models are considerably heavier, usually with more than several hundred thousand finite elements. Each may take more than one day to create and a similar time to run

1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32
33
34
35
36
37
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59
60

(Chen et al. 2018, You et al. 2012).

3.2. Force-displacement curves

To find out whether the alternatives offer a reasonable representation of the overall response of the microstructure or not, the analysis continues towards the force-displacement curves of the grid-divided specimens. These curves show the force sustained by the specimen under displacement (in compression) during the total time of the simulation. Figure 6 presents the force-displacement curves of 100 grid-divided specimens of two microstructures, ‘L1’ and ‘H1’.

Figure 6. Force-displacement curves of 100 grid-divided specimens of two microstructures, L1 and H1, for the three interpolation rules. Curves from 50 to 100 divisions are colored. Notice the difference in vertical scale between specimens.

Clearly, the results of the three interpolations tend to be far from being an accurate representation of the microstructural models. However, an overall consistent behavior is observed, where the three alternatives are converging towards the actual response, and at a medium to high number of divisions, in rules 1 and 3 the force is even within the same order of magnitude as in the original microstructures.

It was expected that the 50/50 interpolation rule would grossly overestimate the stiffness of the grid-divided specimens with few divisions/cells, because every cell with medium to high aggregate fraction would behave as pure aggregate. This was particularly true for the microstructures with high aggregate fraction, as it can be observed that the curves converge towards the real response much slowly for the 'H1' grid-divided specimens than for the 'L1'. However, and perhaps surprisingly, at high numbers of divisions/cells the results obtained from the 50/50 interpolation rule are actually better than the linear approach. Initial results with less divisions/cells are rougher, but shortly after 10 divisions (low aggregate fraction) and around 60 divisions (high aggregate fraction), the force-displacement curves from the 50/50 rule are effectively better approximations to the real response than the linear. At 100 divisions, 50/50 results for the low aggregate fraction are even closer to the actual response than the exponential, which offered the best approximation overall. In general terms, while a perfect fit is not obtained, it is interesting to note that such a coarse simplification is still capable, to a point, of representing the results of the original microstructure.

While the results from the linear interpolation are more consistent than the '50/50', they fail to approach the actual response at an acceptable rate. At 100 divisions, this alternative is the farthest of the three from the microstructural results. Interpolating linearly effectively overestimates the contribution of the aggregates to the mechanical response of the cells, misrepresenting the overall behavior of the specimen. While this is corrected as the divisions increase, the contribution of the cells does not increase linearly with aggregate fraction, even

1
2
3 384 when it does eventually approach the elastic modulus of the rock. On the other hand, the
4
5 385 exponential interpolation rule is clearly the better alternative of the three. It converges quickly
6
7
8 386 and is consistently closer to the real response than the other alternatives, at low and high
9
10 387 aggregate fractions, even at very low number of divisions/cells. The exponential interpolation
11
12 388 is more effectively balancing the mechanical contribution of the cells, and it properly represents
13
14 389 the viscoelastic behavior that dominates at low aggregate fractions.

15
16
17 390 Figure 7 presents a summary of the 100-division specimens of the six microstructures, for
18
19 391 the three interpolation rules. It can be observed that while the specimens with the same
20
21 392 aggregate fraction yield unique results, their behavior is quite consistent (among specimens
22
23 393 with the same aggregate fraction); for instance, the curves from microstructures L1, L2 and L3
24
25 394 differ in value, but are close together (they have the same aggregate fraction) and differentiated
26
27 395 for each of the interpolation rules.
28
29
30

31 396
32
33
34
35
36
37
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59
60

Figure 7. Force-displacement curves from the grid-divided specimens (100 divisions only) of the six microstructures. Specimens with (a) low aggregate fraction, and (b) high aggregate fraction.

3.3. Force at the end of the simulation

An analysis of the force at the end of the simulation offers an interesting insight of the capabilities of the interpolation alternatives. A summary of the force at the end of the simulation for all six microstructures (L1, L2, L3, H1, H2, H3) and grid divisions (1 to 100) is presented in Figure 8.

Figure 8. Force at the end of the simulation ($t = 0.5$ sec, displacement 0.1 mm) for all grid-divided specimens; six microstructures (L1-2-3, H1-2-3), three interpolation rules (50/50, Linear, Exp.). (a) Low aggregate area, (b) High aggregate area. Notice the difference in vertical scale.

Figure 8 provides a clear view of the behavior of the interpolation rules, and the consistency among the simulations. The results from the 50/50 interpolation have a far greater variability, but together with the linear and exponential approximations, their values are consistent among

specimens with the same aggregate fraction (i.e. L1, L2 and L3; H1, H2 and H3). The results are clearly differentiated between interpolation rules, and the nature of the trends is distinct at low and high aggregate fractions, confirming the dominant influence of this parameter in the mechanical response of the specimens. Overall, among the range of divisions selected in this study (i.e. 1 to 100 divisions of a 100-mm side) the alternatives offered a better approximation to the real response for the microstructures with low aggregate fraction; nevertheless, they converge towards the real response for both low and high aggregate fractions, given enough divisions on the grid.

The increased variability among the specimen results for the 50/50 approach may be related to the fact that a *step* function was used to assign their properties (see Figure 4); i.e. the change between elastic and viscoelastic constitutive behaviors is sudden. Therefore, the response of a cell with 49% aggregate fraction may differ widely from that of a cell with 51% aggregate fraction; on the other hand, the transition between these behaviors is smooth for the linear and exponential interpolation rules.

An interesting trend appears in the linear and exponential interpolation rules. In the linear alternative, the force of the grid-divided specimens with low aggregate area (Figure 8a), has an apparent bi-linear trend with the number of divisions in the grid; it starts at 96 kN for 1 division, decreases to around 90 kN for 20-25 divisions, and then it reaches a local maximum; it decreases more rapidly after this point. The trend for the exponential rule increases from 1 to ~25 divisions, presents a maximum (~16 kN), and then it decreases, approaching the correct value of the microstructures. A similar trend was clearly observed at high aggregate area (Figure 8b) for both linear and exponential rules; there is a peak in the force sustained by the grid-divided specimens at ~40 divisions.

The results suggest an interesting property of the microstructure, which is able to reach a 'maximum potential stiffness' at a certain number (or range) of grid divisions. This value seems

to be dependent on the aggregate fraction of the specimen (higher for increased aggregate fraction), and it is probably related to the ratio of the number of pure aggregate/pure matrix cells in the grid-divided specimen, as well as to the maximum nominal size of the gradation of the microstructures. Additionally, in the exponential alternative at both low and high aggregate fractions, this maximum stiffness was roughly twice the actual response of the microstructure. Results from the 50/50 interpolation rule did not follow this pattern.

4. SUMMARY AND CLOSING REMARKS

A simple method was proposed to model the mechanical response of six microstructures of asphalt concrete, three with low and three with high aggregate fraction. This procedure allows for a rough estimate of the actual response of a microstructure, based only on the mechanical properties of its composing phases.

The surface of the microstructures was divided into cells using grids with a range of 1 to 100 divisions (i.e. 1 to 10,000 cells). The aggregate fraction of the cells was used to estimate their mechanical properties, using three simple interpolation rules between the properties of the asphalt matrix and the rock aggregate: (1) 50/50, either matrix or aggregate, (2) linear interpolation, and (3) exponential interpolation.

The results were consistent among different microstructures with the same aggregate fraction, validating the use of this parameter as part of the three interpolation rules. While the approximations are less accurate for microstructures with 'high' aggregate fraction, the three alternatives converged towards the original microstructural response with an increasing number of divisions in the grid. Overall, the exponential interpolation rule was clearly the best and closest to the actual response of the microstructure. The '50/50' alternative yielded more variable results, but in some conditions it behaved better than the more 'refined' linear rule (low aggregate fraction, medium to high number of divisions). In fact, results suggest that it is

possible to identify a cell-wise threshold for aggregate fraction (i.e., instead of 50% in the 50/50 interpolation rule) to generate simple interpolation rules that adjust better to the microstructural response. Additionally, the linear and exponential alternatives exhibited a local maximum in the force resisted by the grid-divided specimens, at the same number of divisions (25 divisions for low, 40 for high aggregate fraction).

Although the results of this study are an approximation to the real microstructural response, it is remarkable that by using simple interpolation rules between only a couple of points (E_o of the matrix, and Young's modulus of aggregates) it was possible to approximate a behavior that is inherently highly complex, and that is affected by the heterogeneity of the microstructure. Even though the grid-divided specimens lack a microstructure, to some extent their behavior can approximate that of the actual specimens of asphalt concrete, including characteristics such as strain concentrations and 'paths', overall deformations, and resulting force. Note that at no point during the analysis were bulk AC properties inputted into the models.

Potential applications for the methodology presented herein include modelling high volumes of mineral-based materials where micromechanical approaches are not practical due to high computational cost, i.e. full pavement cross-sections. Including microstructural characteristics in such conditions (i.e. aggregates, air voids, and/or cracks and other irregularities in full layers), is currently computationally expensive and may require several millions of finite elements for adequate meshing. The proposed methodology may offer a simplified way to approach these models.

The method of grid division is applicable to any multi-phase microstructure, whether acquired by image analysis (real microstructures) or by a packing or otherwise computational algorithm, random or not (virtual microstructures), and the same approach of calculating aggregate fraction in the cells holds in three dimensions. Instead of modulus, any other property may be estimated (e.g. coefficient of thermal or moisture diffusion, with different interpolation

rules) to model a variety of physical processes. Although the methodology is illustrated herein for intact materials, cohesive damage in AC may be considered by replacing the viscoelastic with a damage-encompassing constitutive behavior. Also, as it was mentioned before, the grid does not need to be composed of squares; uneven shapes, or tessellations like Voronoi could be used as well.

Accurate computational models of multi-phase materials can easily become ‘heavy’; some may take hours or even days to run, using special-purpose servers and supercomputers. In this regard, techniques for ‘de-scalation’ of complexity such as the one presented in this study may prove useful, enhancing computational efficiency while maintaining reasonable accuracy in the results.

5. REFERENCES

- Aragão, F.T.S., Kim, Y.R., Lee, J. and Allen, D.H., 2010. “Micromechanical model for heterogeneous asphalt concrete mixtures subjected to fracture failure”. *Journal of Materials in Civil Engineering*, 23(1), pp.30-38.
- Castillo, D. and Al-Qadi, I.L. 2018. “Importance of heterogeneity in asphalt pavement modeling”. *Journal of Engineering Mechanics (ASCE)*, 144(8): 04018060, 1-13.
- Castillo, D., Caro, S., Darabi, M.K. and Masad, E. 2015. “Studying the effect of microstructural properties on the mechanical degradation of asphalt mixtures”. *Construction and Building Materials*, 93, 70-83.
- Caro, S., Castillo, D., Darabi, M. and Masad, E., 2018. “Influence of different sources of microstructural heterogeneity on the degradation of asphalt mixtures”. *International Journal of Pavement Engineering*, 19(1), pp.9-23.
- Chen, J., Wang, H., Dan, H. and Xie, Y., 2018. “Random Modeling of Three-Dimensional Heterogeneous Microstructure of Asphalt Concrete for Mechanical Analysis”. *Journal of*

- 516 *Engineering Mechanics*, 144(9), 04018083.
- 517 Darabi, M., Abu Al-Rub, R., Masad, E., Huang, C.W. and Little, D. 2011. "A thermo-
518 viscoelastic-viscoplastic-viscodamage constitutive model for asphaltic materials".
519 *International Journal of Solids and Structures*, 48, 191-207.
- 520 Elseifi, M.A., Al-Qadi, I.L. & Yoo, P.J., 2006. "Viscoelastic modeling and field validation of
521 flexible pavements". *Journal of Engineering Mechanics*, 132, 172-178.
- 522 Gamez, A., Hernandez, J.A., Ozer, H. and Al-Qadi, I.L., 2018. Development of Domain
523 Analysis for Determining Potential Pavement Damage. *Journal of Transportation*
524 *Engineering, Part B: Pavements*, 144(3), p.04018030.
- 525 Gruber, I., Zinovik, I., Holzer, L., Flisch, A. and Poulikakos, L.D., 2012. "A computational
526 study of the effect of structural anisotropy of porous asphalt on hydraulic conductivity".
527 *Construction and Building Materials*, 36, 66-77.
- 528 Hart, D.J. and Wang, H.F., 1995. "Laboratory measurements of a complete set of poroelastic
529 moduli for Berea sandstone and Indiana limestone". *Journal of Geophysical Research: Solid*
530 *Earth*, 100(B9), 17741-17751.
- 531 Hernandez, J., Gamez, A. and Al-Qadi, I.L. 2016. "Effect of wide-base tires on nationwide
532 flexible pavement systems: Numerical modeling". *Transportation Research Record: Journal*
533 *of the Transportation Research Board*, 2590, 104-112.
- 534 Kim, Y.-R., Allen, D.H. and Little, D.N. 2005. "Damage-Induced Modeling of Asphalt
535 Mixtures through Computational Micromechanics and Cohesive Zone Fracture". *Journal of*
536 *Materials in Civil Engineering*, 17, 477-484.
- 537 Kim, Y.R., Lutif, J.S., Bhasin, A. and Little, D.N., 2008. "Evaluation of moisture damage
538 mechanisms and effects of hydrated lime in asphalt mixtures through measurements of
539 mixture component properties and performance testing". *Journal of Materials in Civil*
540 *Engineering*, 20 (10), 659-667.

- 541 Kim, Y., Lee, J. and Lutif, J.E., 2010. "Geometrical evaluation and experimental verification
542 to determine representative volume elements of heterogeneous asphalt mixtures". *Journal of*
543 *Testing and Evaluation*, 38 (6), 660-666.
- 544 Kim, Y.R., Souza, F.V. and Teixeira, J.E.S.L., 2013. "A two-way coupled multiscale model
545 for predicting damage-associated performance of asphaltic roadways". *Computational*
546 *Mechanics*, 51 (2), 187-201.
- 547 Masad, E., Muhunthan, B., Shashidhar, N. and Harman, T., 1999. "Internal structure
548 characterization of asphalt concrete using image analysis". *Journal of Computing in Civil*
549 *Engineering*, 13 (2), 88-95.
- 550 Obaidat, M.T., Ghuzlan, K.A. and Alawneh, M.M., 2017. "Analysis of volumetric properties
551 of bituminous mixtures using cellular phones and image processing techniques". *Canadian*
552 *Journal of Civil Engineering*, 44 (9), 715-726.
- 553 Ozer, H., Ghauch, Z.G., Dhasmana, H. and Al-Qadi, I.L., 2016. "Computational
554 micromechanical analysis of the representative volume element of bituminous composite
555 materials". *Mechanics of Time-Dependent Materials*, 20 (3), 441-453.
- 556 Rahmani, E., Darabi, M.K., Little, D.N. and Masad, E.A., 2017. Constitutive modeling of
557 coupled aging-viscoelastic response of asphalt concrete. *Construction and Building Materials*,
558 131, 1-15.
- 559 Shakiba, M., Darabi, M.K., Abu Al-Rub, R.K., You, T., Little, D.N. and Masad, E.A., 2015.
560 "Three-dimensional microstructural modelling of coupled moisture-mechanical response of
561 asphalt concrete". *International Journal of Pavement Engineering*, 16(5), 445-466.
- 562 Underwood, B.S. and Kim, Y.R., 2011. "Experimental investigation into the multiscale
563 behaviour of asphalt concrete". *International Journal of Pavement Engineering*, 12 (4), 357-
564 370.
- 565 Wang, H. and Al-Qadi, I.L., 2008. Comparison between mechanistic analysis and in-situ

- 566 response of full-depth flexible pavements. In *Airfield and Highway Pavements: Efficient*
567 *Pavements Supporting Transportation's Future*, 1-15.
- 568 Wang, H. and Al-Qadi, I.L., 2009. Combined effect of moving wheel loading and three-
569 dimensional contact stresses on perpetual pavement responses. *Transportation Research*
570 *Record*, 2095 (1), 53-61.
- 571 Witthüser, K., Arnepalli, D. and Singh, D.N., 2006. "Investigations on diffusion characteristics
572 of granite and chalk rock mass". *Geotechnical & Geological Engineering*, 24 (2), 325-334.
- 573 Yasar, E. and Erdogan, Y., 2004. "Correlating sound velocity with the density, compressive
574 strength and Young's modulus of carbonate rocks". *International Journal of Rock Mechanics*
575 *and Mining Sciences*, 41(5), 871-875.
- 576 Yokoyama, T. and Nakashima, S., 2005. "Diffusivity anisotropy in a rhyolite and its relation
577 to pore structure". *Engineering Geology*, 80 (3-4), 328-335.
- 578 You, Z., Adhikari, S., and Kutay, E., 2009. "Dynamic modulus simulation of the asphalt
579 concrete using the X-ray computed tomography images". *Materials and Structures*, 42, 617–
580 630.
- 581 You, T., Abu Al-Rub, R., Darabi, M.K., Masad, E. and Little, D. 2012. "Three-dimensional
582 microstructural modeling of asphalt concrete using a unified viscoelastic–viscoplastic–
583 viscodamage model". *Construction and Building Materials*, 28, 531-548.
- 584 Zelelew, H. and Papagiannakis, A.T., 2011. "A volumetrics thresholding algorithm for
585 processing asphalt concrete X-ray CT images". *International Journal of Pavement*
586 *Engineering*, 12 (6), 543–551.