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Published in:
Road Materials and Pavement Design

DOI:
10.1080/14680629.2020.1860804

Published: 03/04/2022

Document Version
Peer-reviewed accepted author manuscript, also known as Final accepted manuscript or Post-print

Please cite the original version:
Manrique-Sanchez, L., Caro, S., Estrada, N., Castillo, D., & Alvarez, A. E. (2022). Random generation of 2D PFC microstructures through DEM gravimetric methods. *Road Materials and Pavement Design*, *23*(4), 925-941. https://doi.org/10.1080/14680629.2020.1860804

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Journal:	*Road Materials and Pavement Design*
Manuscript ID	RMPD-20-05-23.R1
Manuscript Type:	Original Scientific Paper
Keywords:	PFC, DEM, FEM, stone-on-stone contact, gravimetric methods

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Abstract

Computational mechanics has proven to be a useful method to understand and assess the mechanical behaviour and main degradation mechanisms of Porous Friction Courses (PFC) at the microstructural level. However, a common limitation when preparing these models is the difficulty to achieve realistic microstructures. The ideal model to evaluate the mechanical behaviour and the degradation mechanisms of PFCs would use a three-dimensional (3D) geometry of the mixture with realistic aggregate shape, angularity, and gradation. However, these models are computationally expensive and typically related with numerical instabilities. This paper proposes a novel methodology to generate two-dimensional (2D) random PFC microstructures using gravimetric methods through Discrete Element Method (DEM) modelling. The proposed methodology was calibrated to generate coarse aggregates with realistic and controlled morphological properties. The produced 2D microstructures were implemented in the Finite Element Method (FEM) Abaqus® and, after coating the particles with asphalt mortar, they were used to verify that the microstructures were able to reproduce the mechanical response –measured through the dynamic axial modulus– of an actual PFC mixture tested in the laboratory. The results show that the proposed methodology is able to produce microstructures with the same dynamic modulus than an actual PFC mixture at different loading frequencies. Among other applications, this methodology could be used to estimate the mechanical properties of PFC mixtures or to assess the expected performance and durability of any specific PFC under realistic field conditions.

Keywords: PFC, DEM, FEM, random microstructures, stone-on-stone contact, gravimetric methods.

1. Introduction

Porous Friction Courses (PFC) –also called Porous Asphalt (PA) or Open-Graded Friction Courses (OGFC)– are hot mix asphalt materials characterized by having total air void (AV) contents ranging between 15 and 25%, and are mostly placed as thin layers of 2-6 cm over conventional pavements (Kandhal, 2002; Putman and Kline, 2012). Since PFCs are highly permeable, this type of asphalt mixture allows the quick drainage of water under rainy conditions, which enhances user safety conditions and reduces hydroplaning risks (Cooley *et al.*, 2009). Moreover, its open microstructure is also useful in reducing tire-pavement noise pollution (Huddleston *et al.*, 1991).

Considering that computational mechanics models are efficient tools in the evaluation of phenomena that are difficult to assess in the laboratory or in the field, a variety of such models have been developed in recent years to assess clogging (i.e., progressive reduction in the AV content of PFC due to contaminants such as rubber or dust, among others), ravelling (i.e., the loss of aggregates due to the repetitive passing of vehicles that leads to mixture disintegration starting from the surface layer), and other phenomena that can affect the functionally and durability of PFC. Most of these works have used Finite Element Methods (FEM) (Huurman *et al.*, 2010; Zhang *et al.*, 2016; Manrique-Sanchez *et al.*, 2018; Manrique-Sanchez and Caro, 2019), while a few have used a Discrete Element Method (DEM) approach (Alvarez *et al.*, 2010a; Yuan *et al.*, 2020).

Since the mechanical performance of PFC depends mainly on their stone-on-stone contact network (Alvarez *et al.*, 2010a), most computational mechanics models of these materials consider the PFC microstructure as a paramount input parameter of the models. In this context, different three-dimensional (3D) and two-

dimensional (2D) techniques have been implemented to obtain PFC microstructures that could be used as input in these modelling efforts.

Regarding 3D models, three types of approaches have been used to represent the aggregate distribution and geometry of PFC microstructures: i) simplified geometry, ii) randomly-generated geometry, and iii) image-based models. Models with simplified geometry use ordered arrangements of spheres or regular polyhedrons to represent the coarse fraction (i.e., aggregates larger than 1.18 mm) of PFC. This approach was followed, for instance, by Mo *et al.* (2008) to evaluate ravelling in FEM simulations. In the second approach, randomly-generated models use spheres, tetrahedral or hexahedral clumps in DEM to represent aggregate particles with predefined angularity indices (Lu and McDowell, 2007). For example, Yang *et al.* (2017) used randomly-generated models in DEM to represent PFC microstructures composed by aggregates with shapes obtained from X-ray Computer Tomography (CT) images, and proposed a new technique to import those microstructures to FEM. Lastly, image-based models use images of PFC specimens obtained from X-ray CT techniques. These images are exhaustively analysed and processed to reconstruct the 3D PFC microstructure. Yuan *et al.* (2020) used this technique to simulate the response of a PFC specimen subjected to an axial compression test.

Computer 3D generated models (simplified and randomly-generated geometries) allow to control aggregate particle sizes and gradations. However, the morphology of the aggregates and the stone-on-stone contact network of these models might not offer a proper representation of the actual 3D PFC arrangements. In contrast, 3D PFC image-based models have an accurate morphology of the aggregates and aggregate-contact network, but its accuracy depends on the image processing techniques applied and the available computation power to perform complex simulations (Yang *et al.*, 2016). In general, properly defined 3D models would give more accurate results than 2D models; nonetheless, it is paramount to evaluate their higher cost in terms of computational operations and time.

In existing 2D approaches, the microstructure of PFC is generally represented by simplified (i.e., circles or polyhedrons) or imaged-based (i.e., image cuts from X-ray CT) geometries. Mo *et al.* (2007 and 2010) used a simplified PFC microstructure composed of thirty circular aggregates to evaluate ravelling using FEM. In contrast, Huurman *et al.* (2010), Zhang *et al.* (2016), Manrique-Sanchez *et al.* (2018) and Manrique-Sanchez and Caro (2019) used 2D image-obtained PFC microstructures to assess the potential of ravelling and the structural capacity (i.e., dynamic modulus, $|E^*|$) of PFCs using FEM. Although 2D PFC models have proven to be effective in the assessment of different phenomena that impact PFC performance and durability, these simplified geometrical models do not always capture the entire morphological properties and gradation of the aggregates (Dai, 2011; Haft-Javaherian, 2011). This condition can alter the stone-on-stone contact network within the PFC and, consequently, its mechanical behaviour.

The objective of this paper is to develop a novel methodology to generate 2D PFC microstructures that efficiently represent the mechanical behaviour of a 3D PFC mixture, while providing the possibility of conducting simulations at lower computation costs when compared to 3D models with similar geometry. The research hypothesis is that it is possible to formulate a low-cost computational methodology to randomly generate 2D microstructures of PFCs that can better capture the mechanical responses of actual mixtures in comparison to current approaches that use 2D image-based or 3D simplified geometries.

To demonstrate the need to improve existing methods, a set of spheres was used in the initial part of this work to represent the coarse-aggregate particles of a PFC, and to prove that 2D PFC microstructures obtained from images of a 3D sample do not resemble relevant 3D PFC microstructural parameters. Following this, the new methodology to create 2D microstructures is described. This novel technique uses a Microstructure Generator (MG) (Castillo *et al.*, 2015) to randomly produce a set of aggregates with

controlled gradation and morphological properties, and the DEM software LMGC90 –developed by Université de Montpellier (Dubois and Jean, 2003)– to apply gravimetric conditions to such a set of particles. The proposed gravimetric modelling approach to generate 2D PFC microstructures was calibrated by subjecting the sets of aggregates –which were coated with asphalt mortar to represent actual PFC geometries–, to a computational dynamic modulus ($|E^*|$) test using FEM, and comparing the results with actual laboratory test results.

It should be noted that the selected DE software uses a contact dynamics approach (Radjai and Richefeu, 2009), instead of more classical DE algorithms, such as molecular dynamics. Although this DE approach faces some challenges (e.g., it cannot be used to evaluate phenomena related to the particle's stiffness and the algorithm can be difficult to parallelize due to its implicit nature), it allows larger time steps than more conventional DE algorithms (Cundall and Strack, 1979). Also, it is easier to use and calibrate since fewer contact parameters are required. Finally, both contact dynamics and molecular dynamics have shown to provide similar results for stiff particles (Radjai et al, 1997), which is the case of the problem under study (i.e., PFC coarse aggregate particles).

The proposed methodology opens the possibility to conduct probabilistic and statistical studies that would be difficult to pursue using 3D computational models or through experimental work, which will lead to a more comprehensive understanding of the mechanisms that control the response of different types of PFC mixtures when subjected to a variety of field conditions. These efforts, could be used, for example, to improve current PFC design and construction methods or to generate realistic input data as part of the life cycle assessment of these materials.

2. Challenges of 2D image-based PFC microstructures

The most common way to obtain 2D image-based PFC microstructures is by using X-ray CT images of PFC laboratory compacted specimens. This technique has been widely used to model dense-graded hot mix asphalt materials, where the coarse aggregates are embedded in a phase of asphalt mortar (i.e., mixture of asphalt binder and the aggregate particles passing sieve size #16, 1.18 mm (Caro *et al.*, 2008)). However, in the case of PFC mixtures, where the coarse aggregates –typically particles retained in the sieve #4, 4.75 mm– create a 3D contact network, this approach might underestimate their actual stone-on-stone contact network (Manrique-Sanchez and Caro, 2019).

To exemplify how 2D image-based PFC microstructures may misrepresent the stone-on-stone contact network of an actual PFC mixture, a 3D granular microstructure that simulates a simplified aggregate skeleton of a PFC was randomly created using the DEM LMGC90 software. This 3D granular microstructure was used to obtain different image-cuts that simulate the 2D image-based PFC microstructures obtained from X-ray CT applied to PFC specimens.

The 3D granular microstructure was created using a set of 406 spheres that emulates the set of coarse-aggregate particles of a PFC, which complies with the typical PFC mixture gradation presented in Table 1. This set of particles was subjected to gravimetric forces using frictionless particles in order to create a stone-on-stone contact network that was as dense as possible. The final 3D granular microstructure measures 60x60x70 mm, which ensures a representative volume element, since these dimensions are three times the Nominal Maximum Aggregate Size (NMAS) of the PFC mixture (Kim *et al.*, 2010).

Table 1. Gradation selected to represent the PFC mixture (FDOT, 2018).

Sieve	FDOT* Specification Limits	Cumulative pass [%]
19.0 mm (3/4")	100%	100
12.5 mm (1/2")	85% - 100%	92.7
9.5 mm (3/8")	55% - 75%	69.4
4.75 mm (#4)	15% - 25%	22
2.36 mm (#8)	5% - 10%	8.7
1.18 mm (#16)	–	5.7
0.60 mm (#30)	–	4.7
0.30 mm (#50)	–	3.7
0.15 mm (#100)	–	2.1
0.075 mm (#200)	2% - 4%	2.1

**FDOT: Florida Department of Transportation*

A total of six image-cuts were extracted from the 3D microstructure: three image-cuts in the horizontal or X-axis direction and three image-cuts in the transversal or Y-axis direction (Figure 1). Next, the 3D and the 2D image-based microstructures were compared using two basic microstructural parameters:

- Coordination number (CN), defined as the ratio between twice the total number of contacts and the total number of aggregate particles (i.e., the average number of contacts per aggregate particle). Overall, the CN is considered a good indicator of the contact network (i.e., the network of stone-on-stone contacts) of the PFC microstructure. Larger values of this parameter indicate better aggregate connectivity and, therefore, a better mechanical response and higher resistance to disintegration (i.e., resistance to ravelling) (Alvarez *et al.*, 2018), and
- Number of floating aggregates (FA), defined as aggregate particles that have one contact or no contacts, or that do not contribute to the contact network (i.e., do not transfer stresses within the microstructure).

Table 2 summarizes the CN and FA microstructural parameters of the 3D granular and the 2D image-based microstructures. The 3D microstructure presented a CN of 4.59, while the 2D image-base microstructures presented an average CN of 0.085. This means that the CN of the 2D image-based microstructures is, on average, 98% lower than the CN of the 3D system. This difference is mainly due to the fact that 91.5% of the aggregates in the image-based microstructures were FA, as those illustrated in Figure 1b. This behaviour was observed in the six image-based microstructures analysed, proving that 2D microstructures obtained through image cuts tend to underestimate the actual stone-on-stone contact density of a 3D microstructure. It would therefore be expected that if these 2D microstructures were used as part of computational numerical models, their mechanical response would not resemble that of actual PFC mixtures.

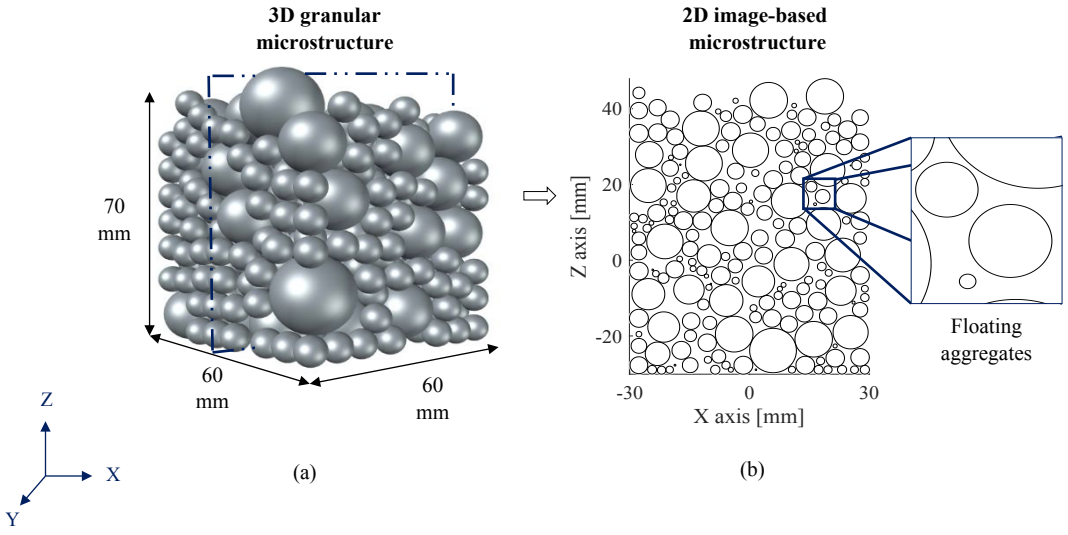

Figure 1. (a) 3D granular microstructure and (b) example of a vertical image-cut obtained from the 3D granular microstructure. The origin of the coordinate system is located at the centre of the 3D granular microstructure.

Table 2. Microstructural parameters of the 3D and 2D image-based microstructures.

Microstructural parameter	3D microstructure		2D image-based microstructures	
	Avg*	Std**	Avg	Std
CN [-]	4.59	N.A	0.085	0.03
FA [%]	6.79%	N.A.	91.47%	3.25%

*Average, **Standard deviation, N.A: not applicable for this case

Considering that these 2D image-based microstructures do to not represent the contact network of a 3D microstructure, the methodology of generating 2D microstructures using gravimetric methods is an interesting alternative. Ten 2D microstructures were generated using the gravimetric method in order to explore whether they could better simulate critical microstructural parameters related to the mechanical response of a 3D microstructure. To do so, frictionless disks aggregates –that followed the gradation presented in Table 1– were randomly located in a predefined space measuring 60x100 mm, as observed in Figure 2a, and subjected to gravity forces using the LMGC90 software, resulting in contact networks such as those presented in Figure 2b.

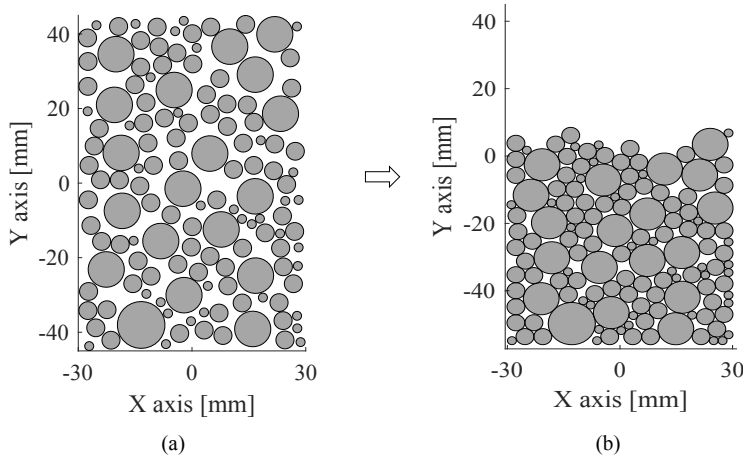

Figure 2. 2D microstructure obtained through gravimetric methods: (a) disk aggregates randomly located and (b) disk aggregates subjected to gravimetric forces.

These 2D microstructures were characterized in terms of their CN and FA and compared with the parameters of the 3D microstructure (Table 3). The results show that the 2D gravimetric microstructures have an average CN value of 3.69, which is 19.5% smaller than the CN in the 3D microstructure. This is similar to the difference between the CN that sphere and disk packings are expected to present in isostatic conditions (i.e., 6 in 3D and 4 in 2D), illustrating that these systems are indeed comparable. In terms of FA, the 2D microstructures obtained through gravimetric methods presented 2.32% FA, while the 3D microstructure presented a total FA of 6.79%. These values are remarkably lower when compared to the average 91.47% FA value obtained in the 2D image-based microstructures. This demonstrates that the 2D microstructures obtained with gravimetric methods have microstructural properties that are closer to those of the 3D microstructure, when compared to the 2D image-based geometries. Thus, it is hypothesized that a properly calibrated gravimetric DEM method would be able to generate 2D microstructures that simulate the microstructural parameters of an actual 3D microstructure and, consequently, would have an equivalent mechanical response. The following section presents the new proposed methodology to generate and calibrate 2D PFC microstructures using the gravimetric DEM method.

Table 3. Microstructural parameters of the 3D and 2D microstructures.

Microstructural parameter	3D microstructures		2D gravimetric microstructures	
	Avg*	Std**	Avg	Std
CN [-]	4.59	N.A.	3.69	0.05
FA [%]	6.79%	N.A.	2.32%	1.36%

*Average, **Standard deviation, N.A**:** not applicable for this case

3. Proposed methodology to generate 2D PFC microstructures

Figure 3 illustrates the general flowchart of the methodology proposed to generate 2D microstructures of PFC mixtures that provide superior simulations of 3D PFC microstructures. This methodology consists in combining three different numerical techniques: i) the MG software (Castillo *et al.*, 2015), ii) the DEM software LMGC90, and iii) the FEM software Abaqus®.

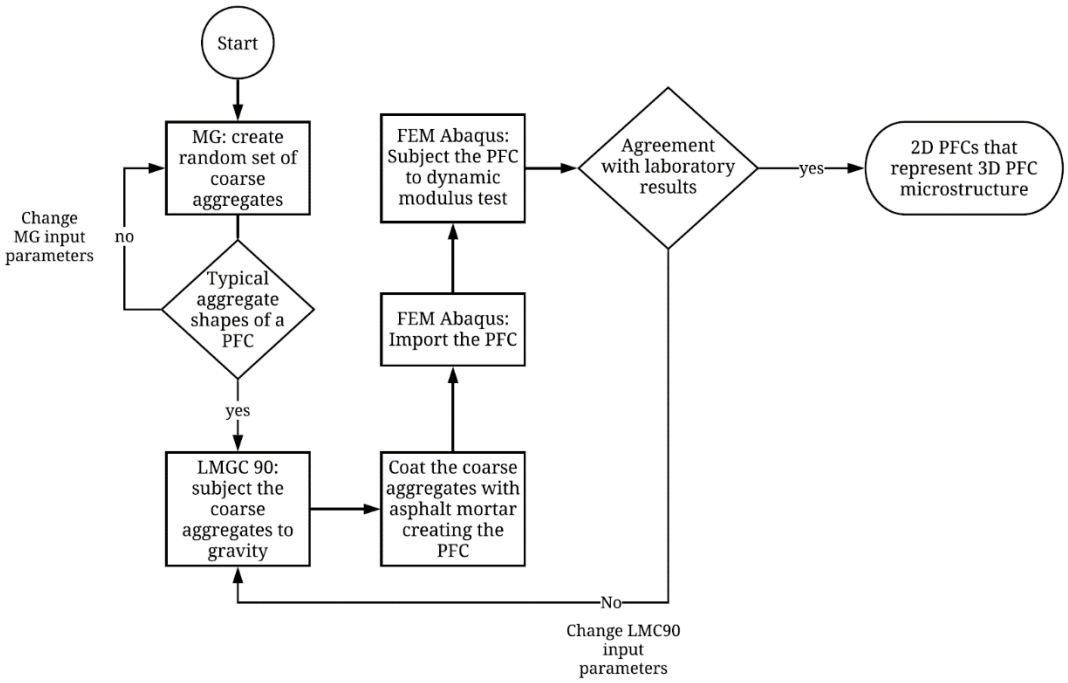

Figure 3. Flowchart of the methodology used to generate and calibrate 2D microstructures of PFC that better represent 3D PFC microstructures.

The MG software is a computational tool that generates random 2D dense-graded asphalt microstructures composed of coarse aggregates that follow specific gradation, orientation, and shape parameters. In this study, the MG software is used to produce sets of coarse-aggregate particles of a PFC mixture with controlled morphological properties. The LMGC90 DEM software is then used to apply gravimetric forces to the set of coarse-aggregate particles generated using the MG. The result of this process is the coarse-aggregate fraction of a 2D PFC microstructure. It is worth mentioning that the final arrangement of the coarse-aggregates depends on the input parameters used in LMGC90, meaning that these parameters need to be calibrated. Finally, the coordinates of the 2D PFC microstructures are imported to the FE software Abaqus®, where the 2D PFC microstructures can be subjected to different mechanical tests after coating each coarse aggregate by a thin film of asphalt mortar. In this case, the PFC mixtures were subjected to computational dynamic modulus tests, or $|E^*|$ tests, to calibrate the mechanical behaviour of the generated 2D PFC microstructures using the experimental results of the PFC mixture used as a reference.

It is important to highlight that the objective of the proposed method is to generate 2D geometries of PFC mixtures with equivalent stone-on-stone networks of actual 3D mixtures, and not to simulate the extension and compaction processes occurring during the construction of these layers in the field. As it will be proven in later sections, the value of this method is that it is a low-cost computational approach that integrates the

MG and DE gravimetric techniques to produce realistic PFC microstructures, without the need of replicating the complex stress conditions induced by field compaction.

Although the methodology proposed in this paper can be used to generate multiple 2D microstructures of any PFC mixture, this work uses a specific PFC to illustrate its different stages. The selected PFC is composed of sandstone aggregates, complies with the gradation presented in Table 1, and uses a neat asphalt binder with 60-70 (1/10 mm) penetration with an Optimum Binder Content (OBC) of 6.5% and a target AV content of 20%. The aggregate gradation and volumetric properties of this mixture were used to conduct the computational generation of multiple 2D PFC microstructures.

In sum, the proposed method uses three different computation tools, and it requires two different calibration processes: i) calibration of the morphological properties of the individual aggregate particles produced by the MG software, and ii) calibration of the input DEM parameters. These processes are described in detail in the following sections.

4. Calibration of the morphological properties of the coarse aggregate particles

The morphological properties of the aggregate particles used in pavement engineering include angularity, form, and texture (Masad *et al.*, 2001; Chandan *et al.*, 2004; Al-Rousan *et al.*, 2005; Singh *et al.*, 2013). Since texture is a difficult parameter to represent in 2D modelling, the MG software does not consider it when generating individual aggregate particles. The angularity and form properties are controlled in the MG software through both the Angularity and Form indexes, or AI and FI, originally proposed by Masad *et al.* (2001) and Al-Rousan *et al.* (2005) respectively, and later adapted by Castillo *et al.* (2018). The AI measures the accumulated change in the orientation of the segments on the perimeter of the particle. Larger values of AI correspond to more angular particles. The AI parameter is calculated by the MG following the equation below (Castillo *et al.*, 2018):

$$AI = \frac{1}{N-1}\sum_{i=1}^{N-1}|G_i - G_{i+1}| \quad (1)$$

where N is the defined number of points located on the 2D perimeter of the aggregate particle and G_i is the orientation of the ith perimeter segment of the particle measured in radians from an arbitrary horizontal line.

On the other hand, FI measures the incremental change in the distance from the geometrical centre to each vertex of the particle in all directions. For example, the FI of a circle is zero and larger values of FI correspond to more elongated particles. The FI parameter is computed using the equation proposed by Masad *et al.* (2001):

$$FI = \sum_{\theta=0}^{\theta=360-\Delta\theta}\frac{|R_{\theta+\Delta\theta} - R_\theta|}{R_\theta} \quad (2)$$

where R_θ is the distance or 'radius' from the centre of the aggregate particle to its perimeter at an angle θ in degrees from the horizontal axis, and $\Delta\theta$ is the increment of the angle at which the perimeter of the aggregate particle would be divided for the analysis. The MG software defines $\Delta\theta$=4°, which means that the perimeter of the aggregate particles is divided into 90 equal sections. To illustrate the influence of the AI and FI

parameters over the final morphological properties of the generated aggregate particles, Figure 4 presents four particles with different AI and FI parameters.

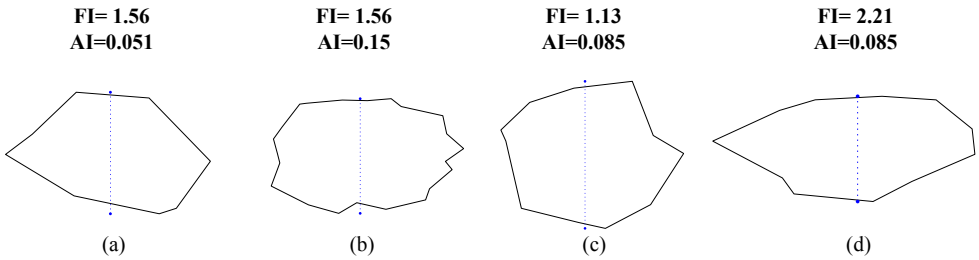

Figure 4. Random aggregates created with different AI and FI parameters: (a) FI=1.56, AI=0.056, (b) FI=1.56, AI=0.15, (c) FI=1.13, AI=0.085, and (d) FI=2.21, AI=0.085.

The MG software controls the final AI and FI indexes of the generated particles using three main parameters: i) the number of vertices of the aggregate particle (*verts: vMin* and *vMax*), ii) the radius from the centre of the particle to the vertices (*r*: *rMin* and *rMax*), and iii) an elongation factor (*elong*), which multiplies the horizontal coordinates of the polygon by a random value '*f*'. The elongation factor creates realistic aggregate particle shapes like those of the aggregates used in asphalt mixtures. The number of vertices follows a uniform probability density function (*pdf*) limited by *vMin* and *vMax;* the radius of the aggregate particles follows a beta *pdf* between *rMin* and *rMax;* and the elongation factor follows a beta *pdf* limited by *f=1* (no elongation) and *f=1+elong*. Once the aggregate particles are created, the MG rotates the coarse aggregates with respect to the horizontal using a factor that follows a uniform *pdf* between -45° and 45°, and randomly locates each aggregate particle in a predefined space. For additional details about the method to control the morphological properties of a set of aggregate particles in the MG software, please refer to Castillo *et al.* (2018).

The parameters indicated above were calibrated in order to obtain aggregate particles with the desired morphological properties of typical PFCs. First, ten vertical images were obtained from two PFC specimens reconstructed using X-ray CT images, since they provide a fair representation of the morphological properties of the aggregate particles. Thus, the AI and FI parameters of a total of 5,148 coarse aggregates were computed and adjusted to the *pdf* that provided the best fit. The best fit for the AI data was a normal distribution, while the best fit for the FI data was a log-normal distribution.

Then, ten sets of 500 aggregates that followed the gradation in Table 1 were created using the MG software. The number of vertices, radius, and elongation factor of these aggregate particles were modified until obtaining *pdf*s of AI and FI that followed the *pdfs* from the image analyses. As a result of the calibration process, the minimum and maximum number of vertices per aggregate were set at 7 and 15, *rMin* and *rMax* were set at 0.38 and 0.6 mm, and the *elong* factor was set at 2.6 (*f=3.6)*. Figure 5a illustrates the normal *pdf* of AI obtained from the images and the fit obtained from the calibration analysis. Figure 5b illustrates equivalent results for FI.

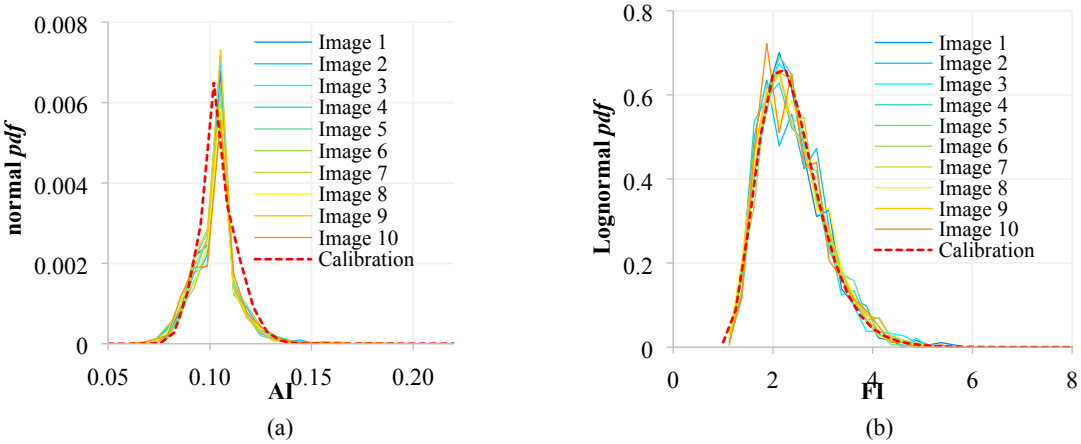

Figure 5. (a) Normal *pdf* of the AI parameter obtained from image analyses and MG calibration, and (b) log normal *pdf* of the FI parameter obtained from image analyses and MG calibration.

5. Calibration of the input DEM parameters and FEM simulations

The LMGC90 DEM software uses the following input parameters for the gravimetric simulation: i) the drop height (*DH*) of the aggregates, ii) the friction coefficient (Φ), iii) the restitution coefficient (i.e., the amount of energy dissipated in collisions) of the aggregate particles, and iv) the density of the aggregates. The microstructural characteristics and, consequently, the mechanical behaviour of the final array of particles depend on these input parameters. As such, the input parameters of the DEM software should be calibrated.

The selected approach for the calibration process consisted in changing the DEM input parameters and subjecting each of the resulting microstructures to a $|E^*|$ computational test in Abaqus®. These computational results were compared to the actual values of $|E^*|$ obtained from PFC samples tested in the laboratory until obtaining similar results.

The experimental results of $|E^*|$, were obtained after testing four cylindrical samples of the selected PFC mixture. The testing specimens were fabricated using the Superpave Gyratory Compactor and their final dimensions were 100mm in diameter and 150 mm in height. Since the internal structure of the PFC mixtures is highly heterogenous (Alvarez *et al.*, 2010b), the PFC specimens were tested twice (once per each side) with a Universal Test Machine MTS, after applying a constant cyclic compressive force of 1,190 N at a frequency of 4, 10, and 16 Hz, following the standard E1876-15 (2015). Table 4 summarizes the $|E^*|$ laboratory results and corresponding statistics.

To initiate the calibration process, three random sets of coarse aggregates with controlled morphological properties were generated using the MG software, using the PFC gradation described in Table 1. The coarse-aggregate particles were randomly located in a predefined space measuring 100 by 300 mm, as shown in Figure 6.

Table 4. Laboratory results of the $|E^*|$ [MPa].

PFC Specimen	4 Hz	10 Hz	16 Hz
1	1,200	1,477	1,506
2	1,363	1,667	1,606
3	1,367	1,669	1,738
4	1,247	1,504	1,536
Avg*	1,294	1,579	1,596
Std**	118	148	176
COV***	9.1%	9.3%	11.0%

*Average, **Standard deviation, *** Coefficient of variation

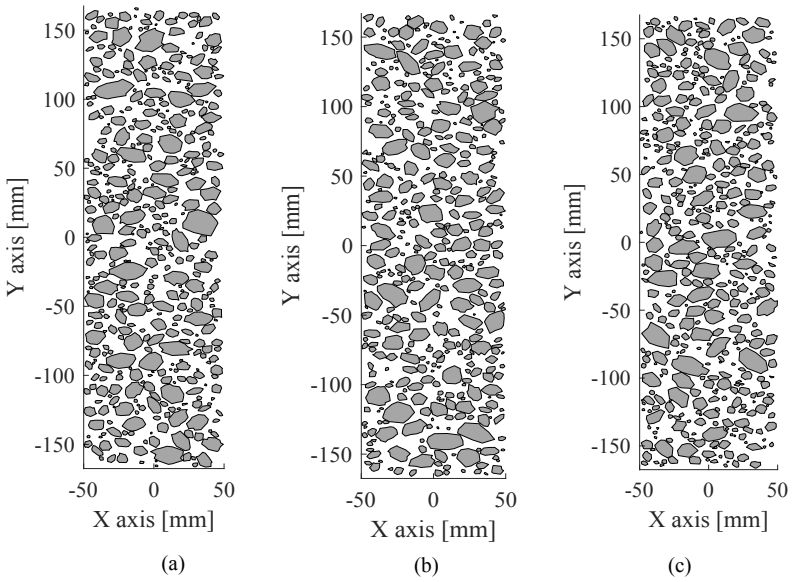

Figure 6. (a) First, (b) second, and (c) third set of coarse-aggregate particles created using the MG software for the calibration process of the gravimetric method to produce 2D PFC microstructures.

The three sets of coarse aggregates were imported into the LMGC90 software, and the Φ and *DH* variables were modified during the application of gravimetric forces. Only these two variables were modified since previous studies determined that these were the most influential factors in the final microstructural characteristics of 2D PFC microstructures (Torres and Caro, 2016; Manrique-Sanchez et al., 2020). Four different Φ values (i.e., 0 (frictionless), 0.35, 0.40, and 0.70) and three *DH* values (i.e., 0, 10, and 15 mm) were selected for the analysis. The restitution parameter was set at 0.3, while the density of the aggregates was set initially at 1,000 kg/m^3, as suggested by Torres and Caro (2016). Notice that this and other bulk properties were assigned to the materials in the DE and, later on, in the FE simulations. Although using 3D bulk properties in 2D simulations is a simplification to the actual problem, is considered acceptable for the scope of this work.

The combination of the Φ and *DH* values resulted in 36 different microstructures with dimensions of 100 by 150 mm. As an example, Figure 7 shows four microstructures created after subjecting the third set of aggregate-particles in Figure 6 to gravimetric forces at a *DH* of 15 mm and at the four Φ values assessed. As illustrated in this figure, although the four resulting microstructures used the same set of aggregate

particles and a constant *DH* value, their internal microstructural parameters, such as the AV content, are different.

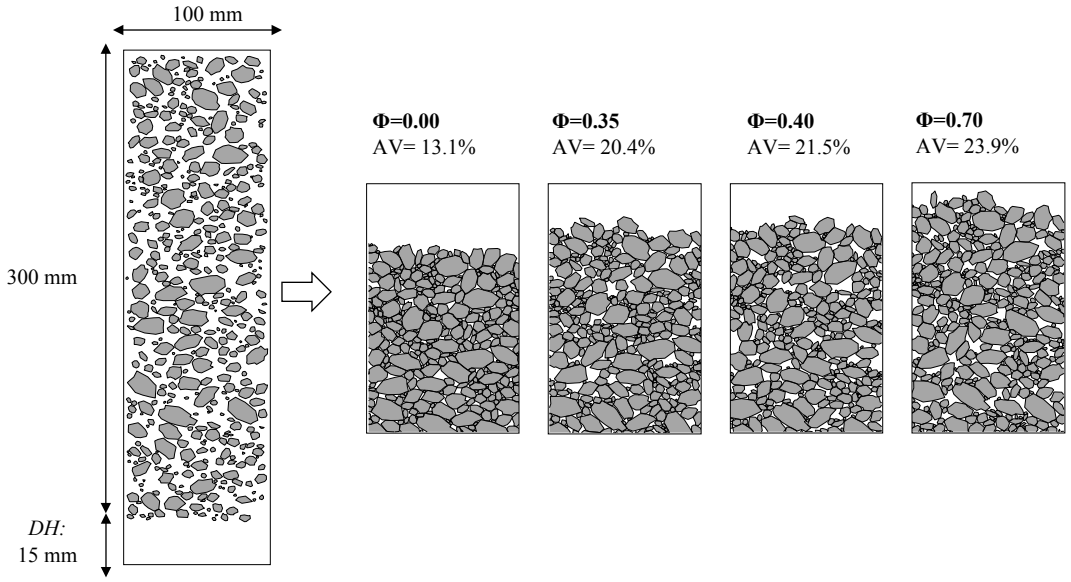

Figure 7. Resulting microstructures obtained with the third MG random set of coarse-aggregate particles with a *DH* of 15 mm, and Φ values of 0.00, 0.35, 0.40, and 0.70.

The coordinates of the 36 PFC microstructures generated with the different DEM input parameters were then imported to the FEM software Abaqus®. The PFC microstructures modelled in Abaqus® have three main components: i) coarse aggregates, ii) asphalt mortar, and iii) air voids. The asphalt mortar uniformly coats each aggregate particle. The thickness of this film was estimated numerically using the gradation and optimum binder content of the PFC mixture of reference, and after assuming a uniform film thickness in all particles, resulting in a value of 60 μm. Figure 8 illustrates the three material components of the 2D PFC models.

In terms of the mechanical response of these components in the FE model, the coarse aggregates were considered linear elastic isotropic materials with a young modulus of 10,000 MPa (Blair, 1955) and a Poisson's ratio (ν) of 0.25. The asphalt mortar was modelled as a linear viscoelastic isotropic material. The rheological properties of the mortar were obtained after applying frequency and temperature sweep tests to small cylindrical testing specimens measuring 125 mm in diameter and 500 mm in height using a solid geometry in a TA200ex rheometer. The details of the fabrication of this type of asphalt mortar samples can be found elsewhere (Caro *et al.*, 2012, 2015). The dynamic modulus results were transformed from the frequency to the time domain to determine the Prony series of the relaxation modulus of the material. The Prony series representing the shear relaxation modulus of a viscoelastic material is expressed as (Fabrizio and Morro, 1992):

$$G(t) = G_{\infty} + \sum_{i=1}^{n} G_i \cdot e^{-\frac{t}{\rho_i}} \qquad (3)$$

where $G(t)$ corresponds to the shear relaxation modulus, G_∞ is the long-term equilibrium modulus, G_i is the i^{th} Prony series parameter, t is time, and ρ_i is the i^{th} relaxation time. The Prony series parameters of the PFC asphalt mortar used in the FE models at a temperature of 25°C are listed in Table 5.

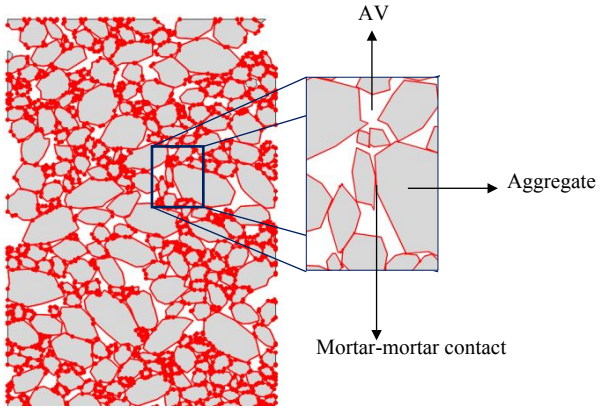

Figure 8. Materials in the FE model of a PFC microstructure generated through the gravimetric method.

Table 5. Prony series of the refence PFC asphalt mortar at 25ºC.

i	ρ [s]	G [Pa]
1	0.01	$1.37x10^{9}$
2	0.10	$4.13x10^{8}$
3	1	$3.13x10^{8}$
4	10	$1.00x10^{5}$
5	100	$8.51x10^{4}$
6	1,000	$9.85x10^{3}$
7	10,000	$9.98x10^{2}$
8	100,000	$1.00x10^{2}$
9	1,000,000	$1.00x10^{1}$
10	10,000,000	$1.00x10^{-1}$
11	100,000,000	$1.00x10^{-2}$
12	1,000,000,000	$1.00x10^{-3}$
13	10,000,000,000	$1.00x10^{-4}$
	G_0 [Pa]	$2.10x10^{9}$
	v [-]	0.40
	G_∞ [Pa]	800

Figure 9a presents a typical FEM model, where it can be observed that the displacement was fully restricted at the bottom of the PFC microstructure, and Figure 9b illustrates the global mesh used in the models. After conducting a sensitivity analysis of the mesh size, the coarse aggregates were meshed using a seed of 15 mm and the mortar was meshed using a seed of 0.75 mm. The coarse-aggregate particles were discretized using 3-node linear elements (i.e., type CPE3R in Abaqus®) and the mortar was discretized using 4-node bilinear elements (i.e., type CPE4R in Abaqus®). On average, a total of 67,000 elements were used per model, a considerably smaller number of elements when compared to a 3D model with similar aggregate geometry.

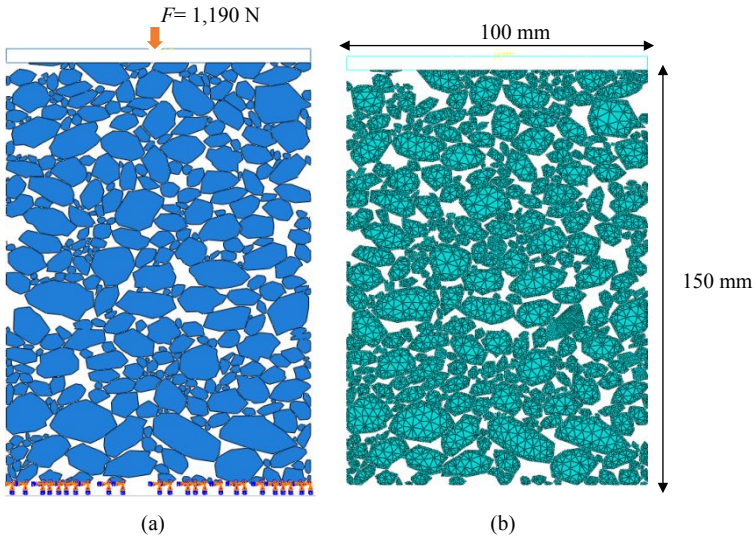

Figure 9. FEM PFC model geometry to obtain their dynamic modulus: (a) load and boundary conditions, and (b) global mesh.

The resulting value of $|E^*|$ was computed based on the amplitude of the stress and strains signals. After conducting all the PFC FEM simulations, several correlations between some microstructural parameters of the PFCs and the resulting $|E^*|$ were analysed. The selected microstructural parameters were:

- AV content
- FA; which in this case also included those aggregates that do not transmit stresses even when in contact with other particles.
- CN, without considering aggregates classified as FA.
- Average length of the contacts between aggregates (ACL), computed as the ratio between the total length of the contacts between aggregates and the number of aggregates.
- The principal orientation of the normal vectors of the contacts (θ_N). The orientation of the normal vector of each contact was computed counter clockwise from the horizontal axis. The principal orientation of the normal vectors of the contacts was defined as the average of all the orientations of the normal vectors within the contacts. The relevance of this parameter is that it influences the load path of two connected aggregate particles (Chang and Lio, 1994).

Figure 10 illustrates the Von Mises stress (i.e., equivalent stress) path distribution of four out of the 36 different 2D PFC microstructures tested at a frequency of 10 Hz. These microstructures were obtained for the first set of aggregates (Figure 7a) by varying the Φ values (i.e., 0, 0.35, 0.4, and 0.7), after maintaining a constant *DH* of 0 mm. This figure shows that as the Φ parameter increases, the AV content increases,

directly affecting the stress path distribution and the |*E**| of the PFC microstructures. In addition, Figure 11d highlights a set of floating aggregates.

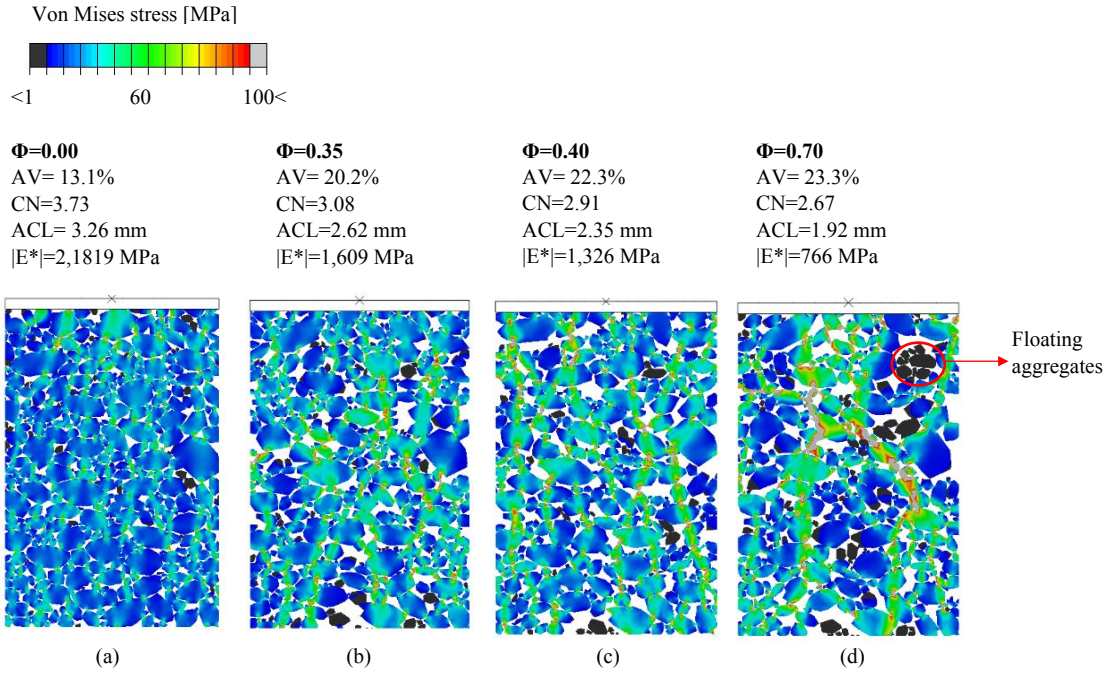

Figure 10. Stress path distribution of four PFC microstructures. The PFC microstructures had a *DH* of 0 mm and Φ coefficients of: (a) 0.00, (b) 0.35, (c) 0.40, and (d) 0.70.

Figure 11 presents the correlation between the selected microstructural parameters and the values of |*E**| obtained at 10Hz. It should be highlighted that floating aggregates were not considered in the computation of CN, ACL, and θ_N. It was found that, in all cases, there is an inverse linear correlation between the |*E**| and the AV content (Figure 12a), while there is a direct correlation between the |*E**| and the CN and ACL (Figure 12b and c). In contrast, it was found that there is no correlation between the |*E**| and θ_N (Figure 11d). Notice, however, that this parameter was not directly modified during the generation of the PFC microstructures, and that it resulted to be similar among all microstructures. Since the θ_N influences the load path of two connected aggregate-particles and the PFC microstructures are usually subjected to vertical loads, an average θ_N of 90°, like the one obtained in this work, is desired. It was also found that there is an inverse linear correlation index of 0.99 between the CN and AV content. These correlations are in good agreement with previous works (Alvarez, Mahmoud, *et al.*, 2010; Manrique-Sanchez and Caro, 2019), and they further corroborate that the mechanical performance of PFCs depends on their geometrical microstructural parameters. It is noteworthy that the correlations presented in Figure 11 could be used as a guide to calibrate the mechanical responses of different PFCs.

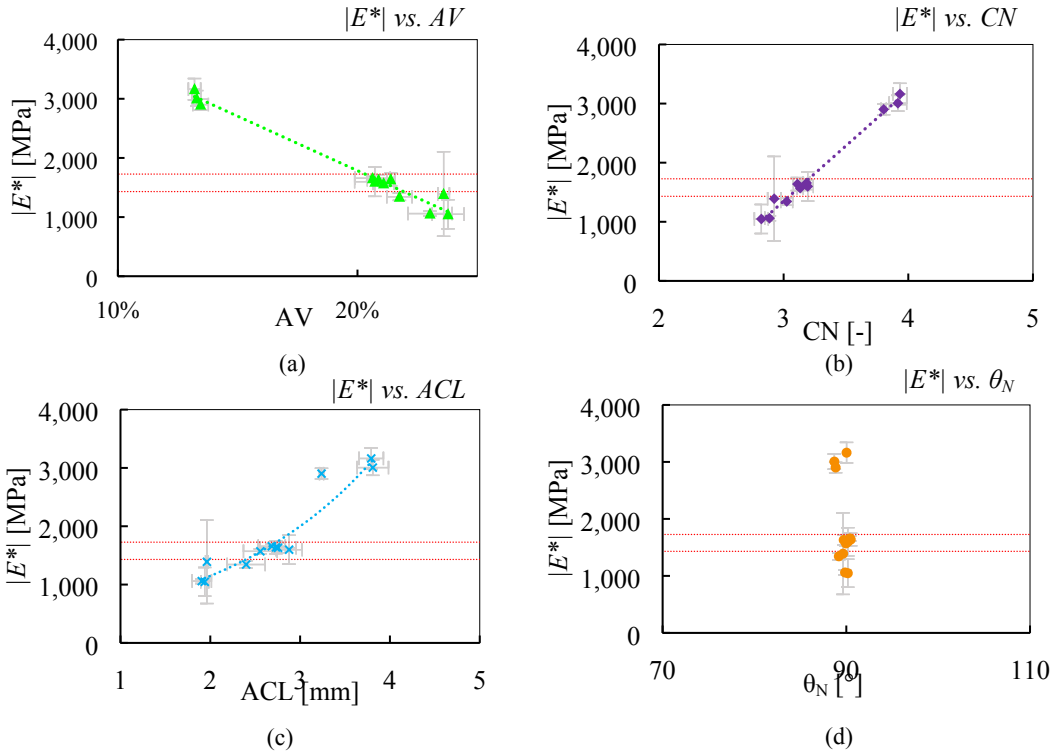

Figure 11. Relationship between the $|E^*|$ and their microstructural parameters evaluated: (a) AV content, (b) CN, (c) ACL, and (d) θ_N. Space within the read lines indicate the average $|E^*|$ at a frequency load of 10 Hz obtained in the laboratory tests.

Table 6 summarizes the average computational $|E^*|$ of the resulting 2D PFC microstructures using the three sets of initial coarse aggregates (Figure 7) with different values of Φ and *DH* during the gravimetric simulations. These results correspond to a loading frequency of 10 Hz. Values in bold and italics in this table correspond to Φ and *DH* combinations that produce PFC microstructures that successfully represent the mechanical performance of the samples tested in the laboratory at 10 Hz (i.e., $|E^*|$= 1,579±148 MPa). It must be noted that intermediate contact frictions (e.g., 0.35 and 0.4) are close to the friction coefficient between real particles (Mitchell and Soga, 2005).

Table 5. Average FE results of the $|E^*|$ [MPa] at a load frequency of 10 Hz.

	$\|E^*\|$ [MPa]					
	DH					
	0 mm		**10 mm**		**15 mm**	
Φ	**Avg***	**Std****	**Avg**	**Std**	**Avg**	**Std**
0.00	2902	92	3006	133	3162	180
0.35	***1657***	***44***	***1598***	***248***	***1630***	***86***
0.40	1344	62	***1638***	***110***	***1570***	***42***
0.70	1047	246	1390	715	1060	42

*Average, **Standard deviation

Table 6 shows that PFC microstructures generated with a Φ coefficient of 0.35 and *DH* values of 0, 10, and 15 mm and those generated with Φ coefficient of 0.4 and *DH* values of 10 and 15 mm resulted in values of |*E**| similar to the experimental result at 10 Hz with a small variability (COV near 3%) among replicates. In general, these PFC microstructures have an average AV content of 20.9% –which correspond to the target AV content of the PFC mixtures evaluated in laboratory–, an average CN of 3.16, and an ACL of 2.72 mm (Figure 13). Nevertheless, to conclude that these sets of input parameters are correct, the numerical |*E**| results at other frequencies should also coincide with the experimental results at other loading conditions. Therefore, the PFC microstructures obtained with these combinations of Φ and *DH* were tested in FEM again at loading frequencies of 4 and 16 Hz.

The data in Table 7 show that the only PFC microstructures that match the experimental modulus at these frequencies correspond to the combination of 0.4 for Φ and 15 mm for *DH*. The PFC microstructures generated with these input parameters had average |*E**| values that were 13.5%, 0.6, and 0.7% higher than the experimental |*E**| values at 4, 10, and 16 Hz, respectively. Considering the heterogeneity of the contact network of the PFC mixtures and the acceptable differences between the numerical and experimental results, particularly for frequencies equal to or higher than 10 Hz, it can be concluded that it is possible to generate random 2D PFC microstructures using DEM gravimetric methods with similar mechanical responses as that of actual PFC mixtures.

Table 7. Average FE results of the |*E**| [MPa] of PFC microstructures generated with Φ=0.4 and *DH*=15 mm at a load frequency of 4, 10, and 16 Hz.

	|*E| [MPa]**		
	Frequency load		
Initial coarse aggregate set	**4 Hz**	**10 Hz**	**16 Hz**
1	1,426	1,527	1,543
2	1,517	1,611	1,625
3	1,465	1,571	1,586
Avg*	1,469	1,570	1,585
Std**	46	42	41
COV***	3.1%	2.7%	2.6%

*Average, **Standard deviation, *** Coefficient of variation

Overall, the results demonstrate that the methodology proposed to generate random 2D PFC microstructures through gravimetric methods can –in terms of computational and time costs– efficiently represent the 3D stiffness at different loading frequencies applied to PFC mixtures. The value of this methodology is that it can be used to generate multiple random PFC microstructures in order to conduct computational probabilistic and statistical studies on the mechanical response of PFC mixtures under different field conditions, a task that would be expensive or even impossible to perform in the laboratory, in the field or with full 3D models.

6. Conclusions

This paper reports a novel methodology to randomly generate 2D PFC microstructures that are able to capture the mechanical response of actual 3D PFC mixtures. Initially, it was demonstrated that the geometries obtained from 2D cuts of 3D microstructures provide inaccurate internal contact networks.

Thus, a novel 2D method was proposed that combines the MG software, to generate random coarse-aggregate particles with controlled morphological properties, and the LMGC90 DEM software, to generate the coarse-aggregate fraction of 2D PFC microstructures using gravimetric techniques. The resulting 2D arrays of coarse-aggregate particles were then coated by a film of asphalt mortar, imported to the FEM software Abaqus®, and subjected to computational $|E^*|$ tests. The resulting moduli were compared against experimental results obtained from the reference PFC mixture. It was found that after a proper calibration process, the DEM model produces microstructures with $|E^*|$ values that produce an acceptable match for the experimental results for the three different load frequencies evaluated (4, 10, and 16 Hz).

Depending on the problem under consideration, a similar approach could be used to calibrate other mechanically-related properties of these mixtures. Overall, these results demonstrate that the proposed technique is a powerful tool to generate random 2D PFC microstructures. This methodology can be used to produce multiple random microstructures of any PFC mixture to conduct computational probabilistic and statistical studies of its mechanical response and degradation, under a variety of field conditions. In particular, the authors will use these 2D PFC microstructures to evaluate the ravelling susceptibility of PFC mixtures using FEM with realistic field operational conditions (e.g., different traffic speeds, load magnitudes, temperature conditions, etc.). Another practical application of this tool is the assessment of the mechanical response of different design approaches for PFC mixtures, after considering the uncertainty induced by the heterogeneity of the PFC microstructures (i.e., computational analysis of multiple randomly generated PFC microstructures as part of reliability-based design approaches).

7. Acknowledgments

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8. References

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Responses to the reviewers' comments

Random generation of 2D PFC microstructures through DEM gravimetric methods

Manuscript ID RMPD-20-05-23

The authors appreciate the comments provided by the reviewers. Next, please find next detailed responses to these comments.

Reviewer 1:

Recommendation: Accept, only if required revisions are made

Comments:

1. Interesting paper on numerical analysis but I am skeptical on practical effect of this work – how this can be used to improve practice-based observations and experience?
   Too much stress on the specific software
   Please clearly state the objectives of your paper and related hypotheses

Response: we appreciate the comments of the reviewer. As any numerical approach, the methodology herein presented is a tool that can be used for multiple purposes. Among other applications, it can be used to: 1) understand and assess the mechanical properties and resistance of PFCs, 2) identify the mechanisms that impact the durability of these layers (e.g., raveling or rutting); this will, in turn, provide information to improve construction methodologies, construction quality control procedures or the use of these materials under specific operation conditions (i.e., corroborating existing field observations and knowledge gained by experience or identifying new relevant aspects), and 3) evaluate the impact of mix design techniques (e.g., gradation, binder content, air void content) on the mechanical properties and durability of the mixtures.

Some of these applications were already mentioned in the introduction, at the end of section 5 and in the conclusion sections. To better emphasize the potential practical applications, additional text on this topic was included in the abstract, introduction and in the conclusions section of the manuscript. It should be noted, though, that the potential applications mentioned are similar to those of published works presenting numerical efforts to evaluate the response of PFCs.

"The application of the proposed methodology opens the possibility to conduct probabilistic and statistical studies that would be difficult to pursue using 3D computational models or through experimental work that will lead to a more comprehensive understanding of the mechanisms that control the response of different types of PFC mixtures when subjected to a variety of field conditions. These studies, in turn, could support improvements in current PFC design and construction methods,"

"Depending on the problem under consideration, a similar approach could be used to calibrate other mechanically-related properties of these mixtures. Overall, these results demonstrate that the proposed technique is a powerful tool to generate random 2D PFC microstructures. This methodology can be used to generate multiple random microstructures of any PFC mixture to conduct computational probabilistic and statistical studies of its mechanical response and degradation under a variety of field conditions. In particular, the authors will use these 2D PFC microstructures to evaluate the ravelling susceptibility of PFC mixtures using FEM with realistic field operational contions (e.g., different traffic speeds, load

magnitudes, temperature conditions, etc.). Another practical application is the assessment of the mechanical response of different design approaches for PFC mixtures, after considering the uncertainty induced by the heterogeneity of the PFC microstructures (i.e., computational analysis of multiple randomly generated PFC microstructures as part of reliability-based design approaches)."

Regarding the stress on the specific software, please notice that the main objective of this work is to propose a new modeling technique to obtain geometries that properly represent the microstructures of PFCs. The value of this work is that it builds on individual existing numerical tools and properly integrates them to propose a novel modeling methodology. Therefore, the description of the details of the methods are a necessary condition to attain the goals of the work. Reducing these details will impact the possibility that other researchers could implement and/or use the proposed technique.

In terms of the objective and the related hypothesis, the manuscript was modified so that the objective and hypothesis of the work were clearly stated in the introduction.

2. Do gravimetric forces simulate and substitute compaction effort?

***Response*:** these forces simulate a natural arrangement of the particles caused by gravity. Although they do not simulate the complex stress conditions imposed by compaction efforts, the value of the proposed approach is that we are able to generate final PFC geometries that resemble probable particle arrangements as those expected in the field. This was clarified in Section 3 of manuscript, as follows:

"It is important to highlight that the objective of the proposed method is to generate 2D geometries of PFC mixtures with equivalent stone-on-stone networks of actual 3D mixtures, and not to simulate the extension and compaction processes occurring during the construction of these layers. In fact, the value of this method is that it is a low-cost computational approach that integrates the MG software and DE gravimetric techniques to produce realistic PFC microstructures, without the need of replicating the complex stress conditions induced by field compaction."

3. This is plenty of numerical manipulations… Such an approach is good for academic exercise but I hope Authors discuss somewhere the practical aspects and consequences of their study

Response: a scientific paper devoted to introduce a computational or analytical method requires plenty of numerical manipulations. As explained in the response to the first comment, the proposed methodology is a powerful tool to understand the response of PFCs and, consequently, to perform computational probabilistic and statistical studies on the functionality, durability and mechanical response of PFC mixtures under different field conditions. As an example, we are currently studying the impact of the quality of field compaction of PFCs in the stiffness and raveling durability of these mixtures.

4. Authors use specific number of vertices, images etc. which makes me wonder about randomization and representation. Did Authors perform pre-studies to determine these specific values and assess their effect on the proposed methodology?

Response: yes, we based the calibration methodology of the morphological properties of the individual particles on the findings reported by:

Castillo, D., Caro, S., Darabi, M., & Masad, E. (2015). Studying the effect of microstructural properties on the mechanical degradation of asphalt mixtures. *Construction and Building Materials*, *93*, 70-83.

Castillo, D., Caro, S., Darabi, M., & Masad, E. (2018). Influence of aggregate morphology on the mechanical performance of asphalt mixtures. *Road Materials and Pavement Design*, *19*(4), 972-991.

In these works, the particle orientation and number of vertices are specified. Also, we calibrated the model using indexes obtained from actual aggregates used in PFCs.

5. Table 5 and 6 – please add some measure of typical variation of experimental results. Lack of statistical analysis

Response: results in Table 4 already show that the variability of the experimental results is between 9.1 and 11%. This variability is considered acceptable and matches previous experimental studies. On the other hand, the variability of the numerical results is, as presented in Table 7, approximately 3%. Since the variability of the numerical results is lower than the variability of the experimental results –due to the numerical control on the generation of the structures—we considered the obtained results acceptable. This was emphasized in Section 5.

Reviewer 2

Recommendation: Accept, but consider suggested revisions

Comments:

This is a very interesting study; the objectives are clear, and the methodology is well explained and executed. Starting reading the manuscript, I had some concerns related to 2D DEM approach as a way to avoid 3D DEM involvement. However, the authors succeeded to present a convincing discussion and a strong case for the employment of a 2D DEM. I do support the publication of this manuscript.
I have a few comments, the authors are invited consider:

Response: we appreciate the positive comments of the reviewer.

1. CN is an important microstructural parameter; however the parameters describing the particulate contact orientation structure are not considered; why? Matching CN is not enough to describe the micromechanical properties.

Response: the reviewer is correct. As mentioned in Section 5 of the paper, CN was not the only parameter describing the geometrical properties of the microstructure. In fact, all microstructures obtained through gravimetric methods were characterized in terms of their:

- Air Void content (AV)
- Floating Aggregates (FA); which in this case also included those aggregates that do not transmit stresses even when in contact with other particles.
- Coordination Number (CN), without considering aggregates classified as FA.
- Average length of the contacts between aggregates (ACL), computed as the ratio between the total length of the contacts between aggregates and the number of aggregates.
- The principal orientation of the normal vectors of the contacts (θ_N). The orientation of the normal vector of each contact was computed counter clockwise from the horizontal axis. The principal orientation of the normal vectors of the contacts was defined as the average of all the orientations

of the normal vectors within the contacts. The relevance of this parameter is that it influences the load path of two connected aggregate particles (Chang and Lio, 1994).

For each microstructure, these parameters (i.e., AV, FS, CN, ACL and θ_N) were compared against the numerically-obtained dynamic modulus, in order to identify which had the highest impact on the mechanical properties of the microstructures. The results showed that not only CN but other geometrical parameters were relevant on determining the magnitude of the dynamic modulus of the PFC mixture.

2. The DEM approach overlooks the real fabrication processes of the PFC materials which invariably include mixing and deposition, not mentioning that all particles are coated during the mixing stages; these aspects are not mentioned and they seem to be ignored in the discussion or reduction of the results. Would coating not would modify the particle-to-particle friction coefficients? How would the numerical results would be affected by these considerations?

Response: please refer to the response to comment 2 of Reviewer 1. The gravimetric DE method herein used does not aim at simulating the complex stress conditions imposed in the material during field compaction. There are some computational mechanics efforts that have tried to simulate compaction of actual asphalt mixtures (e.g., Delft University, RWTH Aachen University, University of Illinois at Urbana-Champaign), which require extremely complex numerical approaches. This is exactly the value of the proposed approach: we do not need to use complex numerical techniques to obtain realistic field-compacted PFC microstructures. By calibrating and controlling the initial conditions of the individual sets of aggregates and the parameters of the DE method (orientation and morphology of the individual particles, and drop height and friction of the set of particles), we are able to create final geometries that properly resemble field-compacted PFCs. In order words, the objective of the method is not to simulate the compaction process but to obtain final particle arrangements with realistic stone-on-stone contact networks. Therefore, the reviewer is correct since during actual construction and compaction processes, the particles are coated by asphalt and, consequently, the actual friction coefficients are different from those used here. However, this is not a concern in this work, as our objective is only to develop a method to generate 'geometries' of PFCs and not to model compaction processes. Notice that after completing the initial stage of producing appropriate spatial arrangements of coarse aggregate particles, these sets are imported to Abaqus and each particle is coated with mortar. Therefore, in the FE simulations, we do count with microstructures that simulate realistic PFC mixtures. This was better clarified in Section 3 of the paper.

3. From where is the value of the restitution parameters coming from?

Response: as explained in the manuscript, this value was obtained from a previous work that assessed the sensitivity of this parameter when using gravimetric methods (Torres and Caro 2016). However, an additional work on this topic further corroborated these results (Manrique-Sánchez et al. 2020):

> Manrique-Sanchez, L., Caro. S., Tolosa, D.F., Estrada, N., Castillo, D. (2020). "Challenges in the generation of 2D Permeable Friction Courses (PFC) microstructures". Proceedings of Advances in Materials and Pavement Performance Prediction (AM3P). San Antonio, Texas, USA.

We have added this new reference in the revised version of the paper.

Reviewer 3

Recommendation: Accept, only if required revisions are made

Comments:

1. The manuscript reports on a numerical study using both the Discrete element (DE) and the finite element (FE) method to simulate the dynamic modulus response of a Porous friction course (PFC) mix by taking into account its microstructure at the aggregate scale. As stated in the Introduction section, the manuscript proposes a 'methodology to obtain random 2D PFC microstructures that efficiently represent the mechanical behaviour of a 3D PFC mixture while providing the possibility of conducting simulations at lower computation costs, when compared to 3D models with similar geometry.' The procedure is based on information from 2D, computed tomography images. As the Authors correctly state in Section 2, the characterisation of a granular aggregate microstructure using 2D images has inherent limitations. Namely, the air void content as well as the number of `floating' aggregate particles and the coordination number of the contact network of aggregate particles, as obtained from 2D computed tomography sections, are unrealistic. This quite trivial remark is however clarified by an example, in the same section, on a DE assembly of spherical particles. In Section 3, the Authors outline the procedure which they propose to design 2D DE granular materials whose microstructure and simulated mechanical response be in near quantitative agreement with the real PFC material. Section 4 focuses on how the DE particles were generated according to the morphological characterisation of the aggregate population of the reference PFC material. Section 5 reports on the DEM simulations by which a parametric set of microstructures was obtained, as well as on the FE simulations by which the same model microstructure were submitted to 2D dynamic modulus tests.

   The manuscript is well written, fully understandable, with good quality figures and tables. I do not subscribe to the point of view that 2D modelling is the mid/long term perspective (which is set in my opinion by accurate 3D grain scale measurements as can nowadays be performed from computed tomography scans [doi: 10.1007/s11440-011-0151-6]). However, in my opinion, the study is worth being communicated as an interesting two-dimensional numerical exercise, provided the Authors agree on the minor improvements in following list of remarks.

Response: we appreciate the positive comments of the reviewer and truly appreciate his/her opinions. We do agree that the mid/long term goal is to have 3D microstructural models that could be randomly generated or efficiently reconstructed from images obtained through X-ray CT tomography. In fact, we are aware of the efforts conducted in this direction in the last 10 years by several research groups. However, as explained in the document, the associated computational cost of these approaches is currently too high, which restrains the possibility of conducting multiple simulations (hundreds or even thousands), in order to capture the uncertainty of the mechanical response of these mixtures. This is important, as we personally believe that pavement engineering should move forward to include uncertainty quantification (structural reliability analysis) as part of current design approaches, as it has been already done in structural and geotechnical engineering during the last two decades.

2. The main title should mention that the proposed analysis is two-dimensional.

Response: the title was modified as suggested.

3. DEM/FEM simulations should appear as keywords.

Response: the reviewer is correct. These words were included as keywords, as suggested.

4. The LMGC90 software implements the contact dynamics approach to DE simulations, instead of the more common molecular dynamics approach. In this sense, a quick characterisation of the contact dynamic approach appears to be a necessary piece of information that is currently missing from the numerical background of the study.

Response: the reviewer rises a good point. The contact dynamics of the DE method is a combination of three main components: i) equations of motion, which relate the impulse to the change of momentum of each particle, ii) contact laws, which relate the impulses exerted at each contact with the change of relative velocity during the time step, and iii) the algorithm of solution (i.e., an implicit solution that use an algorithm similar to a Gauss Seidel scheme) (Radjai and Richefeu, 2009). Although the contact dynamics method cannot be used to evaluate phenomena related to the particle's stiffness and the algorithm can be difficult to parallelize due to its implicit nature, it allows larger time steps than more conventional DE algorithms, such as molecular dynamics (Cundall and Strack, 1979). Also, the contact laws do not need to be regularized, which implies fewer contact parameters and, consequently, it eases its use and calibration. Finally, it has been demonstrated that similar results can be obtained with both contact dynamics and molecular dynamics for stiff particles (Radjai et al, 2997), which is the case of the problem under study.

We have now explicitly mentioned in the Introduction that the selected software uses a contact dynamics DE approach, and we have also justified its use over more conventional DE algorithms, as suggested by the reviewer.

5. The current title of Section 5 is not appropriate because the section (i) includes both DEM and the FEM simulations and (ii) discusses also the relevant results (not only the parameters).

Response: we agree with the reviewer. The title of Section 5 was changed to Calibration of the input DEM parameters and FEM simulations.

6. Some parameters of the numerical simulations only catch the relevant orders of magnitude (e.g. 10 GPa for the Young's modulus of the bulk material of the aggregate particles in the FE simulations; see also the following remark). In this sense, and due to the two-dimensional setting, the semi-quantitative character of the proposed analysis should be more clearly acknowledged in the Abstract and in the Introduction section.

Response: we are not positive we fully understood the comment of the reviewer. Even though using bulk properties in 2D simulations imposes some limitations in the precision of the model, it is a common practice in this type of works, and it is considered enough for the purposes of the study. Following the recommendation of the reviewer, we have explicitly acknowledged this in the text (Section 5, after Figure 6).

7. Please clarify the 1kg/mm^3 aggregate bulk density of the DE simulation [p.10, l. 53].

Response: this is a mistake and we are glad the reviewer noticed it. The correct value for the aggregate bulk density is 1000 kg/m^3. This was corrected in the manuscript.

8. Please clarify that the FE modelling refer to linear elastic/viscoelastic ISOTROPIC materials, and that the modulus referred to at p. 11 l. 41 is Young's modulus.

Response: we included these clarifications, as suggested. Thank you.

9. Stress measurements are performed in Pa units : how 3D units are inferred from 2D simulations should not be dismissed as a trivial point (which is not).

Response: the reviewer is correct: this is not a trivial point. We obtained the 2D stress results using a plane stress analysis with an assumed thickness of 10 cm. Even though this is a simplification, the results proved to be in good agreement with the experimental results.

10. At p. 15 l. 5-6 the Authors state that 'there is no correlation between the $|E^*|$ and θ_N, based on Figure 12d. This is a very doubtful inference, as the latter parameter does not vary, actually, in their analysis.

Response: when the set of particles were subjected to gravity forces, the parameters that were controlled were the morphology of the aggregates, the friction among particles and the drop height. We did not directly control θ_N, as this resulted from the final PFC microstructure. The results show that θ_N was not sensitive to the selected modeling approach. However, the reviewer is correct in pointing out that we did not vary this parameter in our analysis, and that the obtained values were equivalent in all microstructures. This was clarified in the manuscript (Section 5, with the discussion of Figure 11).