3D Simulations of Two-Component Mixes for the Prediction of Multi-component Mixtures' Macrotexture: Intermediate Outcomes

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Abstract. It is a consolidated knowledge that road macrotexture affects direct primary aspects related to road safety as friction or aquaplaning and secondary aspects related to environmental issues as noise or fuel consumption. These premises highlight how the prediction of road macrotexture is still an open research field for pavement designer, especially for theoretical models which would better describe the relationships with grading and volumetric properties, laying techniques and compaction energy.

In this paper intermediate outcomes about the theoretical prediction of road macrotexture are presented. In order to investigate the arrangement and compaction of a bituminous mix in a gyratory compactor, the Discrete Element Method (DEM) approach has been used to develop numerical simulations of two-component mixes. A large simulation campaign has been designed and performed and the Void Content diagram has been used for the macrotexture representation.

In analogy with the packing theory, the extension of the results obtained for the two-component mixtures into the multi-component systems, has been proposed and an effective novel theoretical method, based on a "revisiting" of the classical Void Content diagrams, for the macrotexture prediction has been performed. Finally, a numerical application of the method has been provided and the outcomes discussed.

Keywords: Discrete Element Method (DEM) · Packing model · Void Content diagram · Two-component mixes · Numerical simulation · Macrotexture · Road pavement

1 Introduction

Within scientific literature, significant association between low macrotexture and crashes risk have been found [1–3], as well as macrotexture and friction in wet conditions [4] or skid deterioration models [5]. For these reasons the road macrotexture prediction is of prominent interest for both private and public road management agencies. In the past,

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empirical models have been deeply analyzed, their critical issues have been brought to light and tried to overcome [6, 7]. However, further studies are necessary to deeply investigate the theoretical links between the macrotexture and the volumetric and grading characteristics of the bituminous mixtures and the compaction techniques and released energy. This work fits in this direction.

1.1 Field and Laboratory Tests Overview

Both laboratory and outdoor methods are available to measure the macrotexture and the simplest and most known method is the Sand Patch Method [8]. It is a volumetric method that, with a very simple apparatus and test process (see Fig. 1), provides the average pavement macrotexture depth, expresses by means of the Mean Texture Depth (MTD) which, according to the Standard [8] can be evaluated by means of the Eq. (1):

$$MTD = \frac{4 \cdot V}{\pi \cdot D^2} \tag{1}$$

where:

- MTD = mean texture depth of pavement macro-texture [mm];
- V = sample volume [mm^3];
- D = average diameter of the area covered by the material [mm].

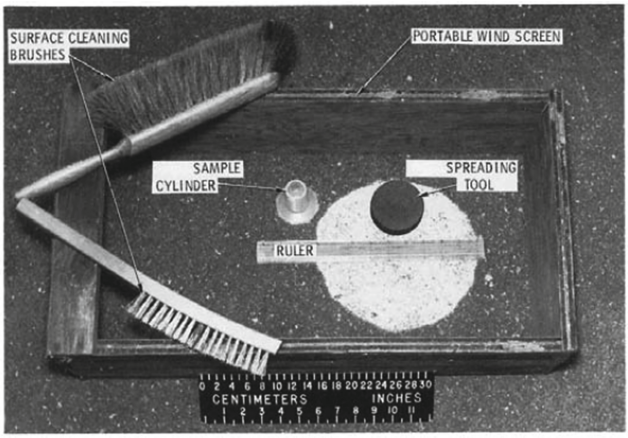

Fig. 1. Apparatus for sand patch measurement [8].

In order to simulate and reproduce the compaction technique under actual road laying operations, with the aim to analyse the final compaction condition of the asphalt in terms of void content, the gyratory compactor has been identified as adequate laboratory test [9]. In fact, the test is able to reproduce on the bituminous specimen, shearing forces similar to those performed under the action of a roller during field compaction [10].

Furthermore, the choice to use the gyratory compactor specimens, well fits with the use of the DEM simulation method, allowing to considerably reduce the computational burden.

1.2 Packing Theory Background

In a non-exhaustive way, a brief introduction on the most important basic concept of aggregate packing has been provided below.

Since the mid-1920s, several studies have been performed in order to investigate factors affecting packing and porosity of cement and asphalt concretes [11–13].

As far as two-component mixtures have been concerned, two types of particles interaction have been highlights:

- The wall effect, due to the interaction between particles and any type of boundary placed in contact with the granular mass;
- The interference effects, due to the increasing fraction of fine aggregates added to the coarse fraction, which cause the coarse-to-coarse contact.

First significant developments of the Void content diagrams have been done by Furnas [11], which on the basis of numerous experiments, produced generalized experimental curves describing the void index variation of the mix, varying both coarse aggregate proportion and diameter ratio of fine and coarse aggregates (see Fig. 2).

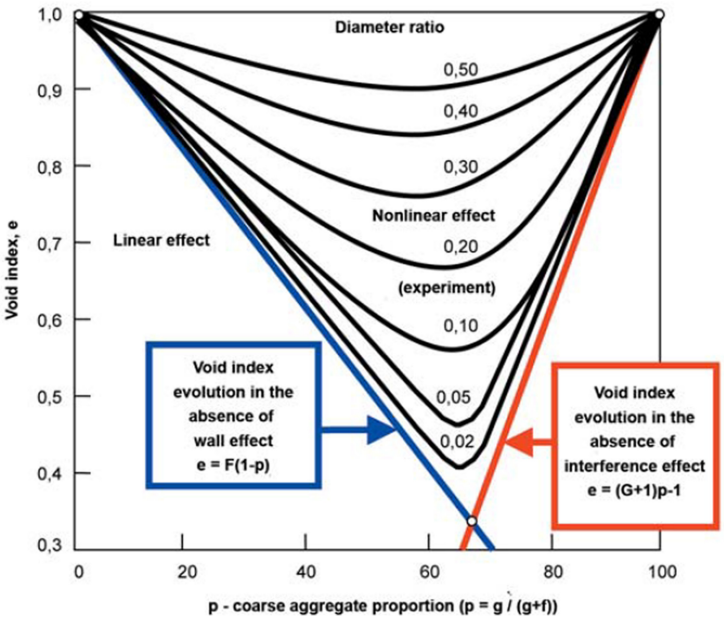

Fig. 2. Void Content diagram of a two-component system of coarse (g) and fine (f) aggregate vs. the coarse aggregate proportion for different diameter ratios [14].

As it is possible to see, according to the experimental evidences, the curves present a clear minimum and for any given proportion of fine to coarse aggregate, the voids in the mix decrease with decreasing diameter ratio.

1.3 Objective

The main aim of this paper is to introduce a novel theoretical method for the macrotexture prediction of multi-component spherical mixtures, by means of the Void Content diagram representation.

Twenty simulations of gyratory compaction specimens, of two-component spherical mixes, with five different fixed fractions of fine particles respect to the coarse particles, have been performed. The macrotexture values have been evaluated and depicted in analogy to the Void Content diagram designed for the representation of the voids ratio of two-component mixes.

Finally, a numerical application of the proposed method has been provided and the results have been discussed.

2 Design of the Virtual Experimental Campaign

2.1 Numerical Model

The Discrete Element Method (DEM) is a numerical method, introduced in 1971 by Peter Cundall [15], in which discrete spherical particles collide one each other and with other surfaces using the force-displacement law. Each particle is represented as a rigid spherical single-node with fixed radius and uniform density and is characterized by 6 degrees of freedom.

With the geometry, the contact behavior, which represents the constitutive behavior of the materials, is the second crucial factor of the DEM simulation. According to the literature [16–19], in order to simulate the rheological behavior of asphalt mixtures, the viscoelastic model called Hertz-Mindlin (H-M) Model, which is composed by two Kelvin's constitutive models, has been used [20].

In order to simulate the real laboratory gyratory compactor test, the numerical model has been designed according to the Standards [9, 10, 21]. The external geometry is composed of the mould, the plate and the funnel. The first two are actually part of the gyratory compactor apparatus, on the contrary, the funnel has been introduced in the simulation, to guaranty an effective random arrangement of the spherical particles, which impact on its internal wall.

In particular the steel mould, plate and funnel have been designed as rigid bodies, with null thickness, meshed with shell elements and characterized with different geometries:

- Mould: cylinder with height (H) of 150 mm, circular internal diameter (D) of 150 mm (inner radius of 75 mm), and compaction angle of 1.25°.
- Plate: circle with diameter (D) of 150 mm.
- Funnel: conical geometry characterized by the smaller radius of 60 mm (Rmin), the bigger radius of 1000 mm (Rmax) and height (Hf) of 1240 mm (required dimensions to guaranty a regular distance between the particles in the initial position).

Their assembly has been reported in the Fig. 3.

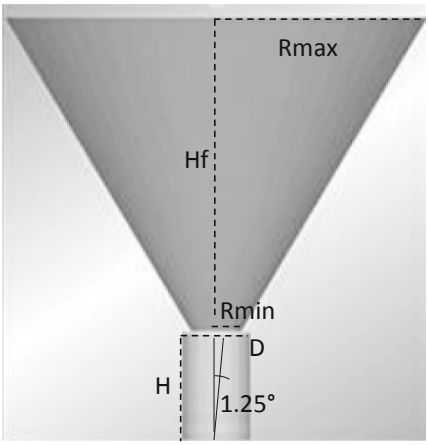

Fig. 3. Virtual model of the gyratory compactor with the funnel.

The aggregates have been represented by rigid bodies with spherical shape, which are characterized by a density of 2500·kg/m^3 and radius between 20 mm and 4 mm. The most important features have been summarized in the Table 1:

Table 1. Features of the virtual particles

Diameter [mm]	Radius [mm]	Volume [mm]	Volume [mm]	Mass [mm]
20	10	4188.79	4.18879E−06	0.010472
16	8	2144.661	2.14466E−06	0.005362
12	6	904.7787	9.04779E−07	0.002262
8	4	268.0826	2.68083E−07	0.00067
4	2	33.51032	3.35103E−08	8.38E-05

As far as the kinematics and loads are concerned, the mould is characterized by a constant rotation of 30 rev/min around the compaction axis (angle of 1.25° respect to the vertical axis), the plate, once that all the spheres have been fallen into the mould, applies a vertical pressure of 600 kPa. Finally, it should be highlighted that, in order to reduce the analysis noise, the mass proportional damping has been used and that the friction coefficient for the contact between particles has been set at 0.5 and between particles and plate/mould at 0.2.

2.2 Previous Findings

In order to establish the better simulation procedures and to calibrate the virtual model, several efforts have been spent within previous virtual and laboratory tests and the main results have been summarized below [20]:

- Repeatability analysis: in order to investigate if the initial position of each sphere, affects the final macrotexture value, 25 simulations with different initial positions of the monogranular mix with 20 mm of diameter, have been performed. It has been demonstrated that the funnel allows an effective arrangement of the particles and, according to the literature [7, 22], the variability of the values of the macrotexture is conserved and the test is repeatable.
- Wall Effect Analysis: due to the dimension of the particles respect to the mould, along the boundary line, the mobility and the compaction of the particles could be more difficult. Although the spheres' dimension is the most important affecting factor, a cut of 15 mm along the boundary of the virtual specimen has been identify to neglect the wall effect, regardless particles' radius.
- Reference Depth: the simulations on the monogranular mixes have shown that the cut at depth 'D/2', respect to the upper surface of the specimen, produces MTD values closer or belonging to the theoretical packing configurations domain (the cubical packing model and the tetrahedral packing model which represent the loose and the dense configurations respectively).

2.3 Simulation Series Design

In order to investigate the behavior of two-component mixtures, especially in terms of compaction and mutual interference, according to the packing theory [11, 13] a set of simulations, with different d/D ratio, has been performed.

With the aim to find a compromise between the results validity and the computational efforts, 20 mm for the maximum aggregate diameter and a duration of 10 s of virtual simulation have been selected and four two-component mixes have been designed, with fixed total mass and density, of about 2,86 kg and 2500 kg/m^3, respectively. For each mixture, five different percentage proportions have been defined: 0%–100%; 25%–75%; 50%–50%; 75%–25% and 100%-0%. The most important features of the mixtures have been summarized in the Table 2:

Table 2. Characteristics of the simulations of the two-component mixtures.

d/D	Incidence				
16/20	0%–100%	25%–75%	50%–50%	75%–25%	100%-0%
N° particles	273	133–204	267–136	400–68	527
N° particles ratio	0	0.651961	1.963235	5.882353	–

(*continued*)

Table 2. (*continued*)

d/D	Incidence				
16/20	0%–100%	25%–75%	50%–50%	75%–25%	100%-0%
Virtual duration sim. [sec]	10	10	10	10	10
Real duration sim. [h]	8	9.5	11	13	15.5
12/20	0%–100%	25%–75%	50%–50%	75%–25%	100%-0%
N° particles	273	316–204	632–136	945–68	1275
N° particles ratio	0	1.55	4.65	13.90	–
Virtual duration sim. [sec]	10	10	10	10	10
Real duration sim. [h]	8	20.5	38	54.5	70
8/20	0%–100%	25%–75%	50%–50%	75%–25%	100%-0%
N° particles	273	1063–204	2126–136	3189–68	4285
N° particles ratio	0	5.21	15.63	46.90	–
Virtual duration sim. [sec]	10	10	10	10	10
Real duration sim. [h]	8	74	131.5	182.5	238
4/20	0%–100%	25%–75%	50%–50%	75%–25%	100%-0%
N° particles	273	8531-204	17063-136	25594-68	34125
N° particles ratio	0	41.82	125.46	376.38	–
Virtual duration sim. [sec]	10	10	10	10	10
Real duration sim. [h]	8	413	645	848.5	1080

By way of example, the d4/D20 two-component mixtures with the three percentage proportions, before the compaction phase, have been showed in the Fig. 4.

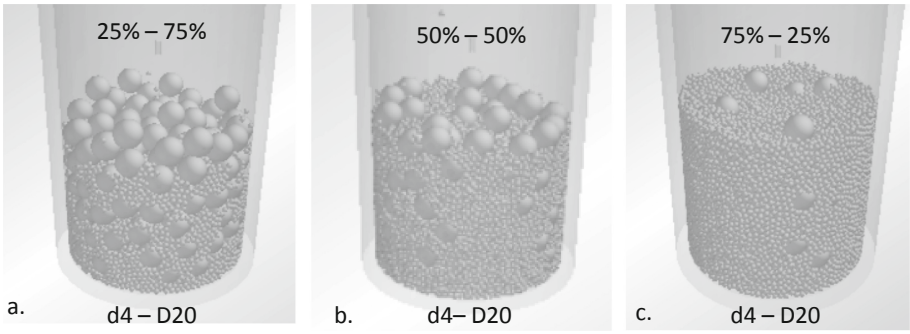

Fig. 4. Random arrangement of the two-component mixture d4/D20, before the compaction phase, with the percentage proportions: a. 25%–75%; b. 50%–50%; c. 75%-25%.

Although the entire development of the simulation has been previously detailed [20], a brief general description of the individual steps of the virtual test is provided. The simulation is composed of four phases:

1. Definition of the position of the apparatus (mould, plate and funnel) and of the particles in a regular grid;
2. Free fall of the particles into the funnel and consequently into the mould;
3. Right position of the plate into the mould;
4. Rotation of the mould around the compaction axis at 30 rev/min, and compaction of the plate to the mixture with a vertical pressure of 600 kPa.

2.4 Post Analysis of the Outputs

In order to evaluate, for each simulation, the final value of the macrotexture, in terms of MTD index, the construction of the upper surface of the virtual specimen, by means of an ad hoc code, has been performed. In particular the code allows to distinguish the size of each particle and to convert the coordinates of the node (x, y and z) into a grid-surface with a sample spacing of 0.5 mm. The flowchart of the conversion procedure has been summarized in the Fig. 5.

It must be observed that the Deq (equivalent diameter in terms of volumetric properties) can be considered a theoretical dimension of the virtual particle if the two-component mix would be composed of only one fraction. Its evaluation has been reported in the Eq. (2).

$$D_{eq} = \sqrt[3]{\%_D \cdot D^3 + \%_d \cdot d^3} \tag{2}$$

where:

D_{eq} is the equivalent diameter of the corresponding monogranular mix;
$\%_D$ is the percentage of the larger fraction respect to the total mass;
D is the diameter of the larger particle fraction;
$\%_d$ is the percentage of the fine fraction respect to the total mass;
d is the diameter of the fine particle fraction.

For all the 20 simulations introduced in the Table 2, the procedure summarized in the Fig. 5 has been applied selecting 13 fixed temporal steps: 1.5 s, 2 s, 2.5 s, 3 s, 3.5 s, 4 s, 4.5 s, 5 s, 6 s, 7 s, 8 s, 9 s, 10 s. In fact, as demonstrated [20] within 0 to 1.5 s the mixtures stabilize.

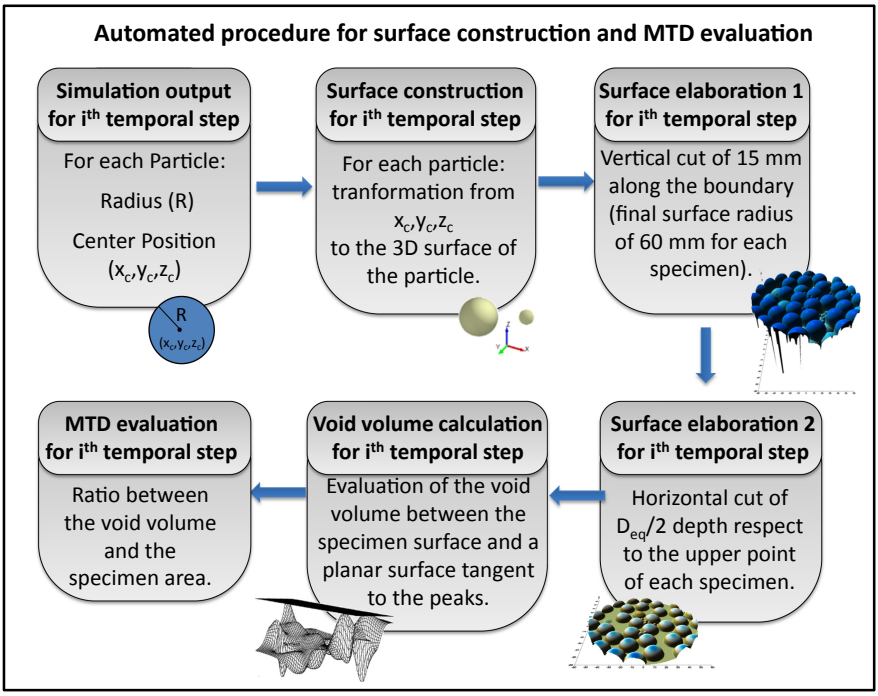

Fig. 5. Workflow of the automated procedure for the construction of the surface specimen and MTD evaluation.

By way of example, with a fixed percentage proportion of 50%–50% the final surfaces of the two-component mixtures d16-D20, d12-D20 and d8-D20, have been reported in the Fig. 6.

Finally, 260 final surfaces have been constructed and their relative MTD values have been evaluated.

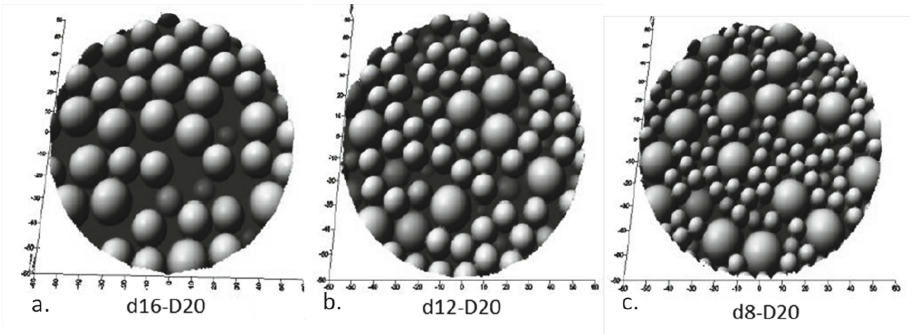

Fig. 6. Deq/2 surface with the final surface radius of 60mm of the mixtures with the percentage proportion of 50%–50% and with the d-D ratios a. 16–20; b. 12–20; c. 8–20.

3 Analysis of the Results

3.1 Time History Analysis of the Two-Component Mixtures

According to the physical sense and to the outcomes observed in the time history analysis of monogranular mixtures [20], the macrotexture, expresses by means of the MTD value, follows a decreasing trend. This evidence is summarized in the Fig. 7 where, by way of example, three different mixtures have been selected.

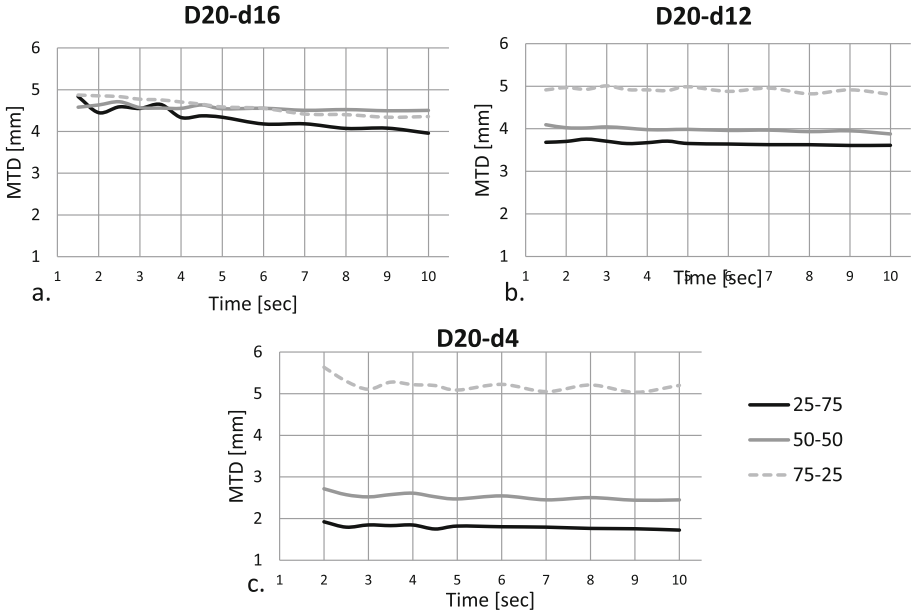

Fig. 7. Time history curves at different level of percentage proportion for the mixtures a. 16–20; b. 12–20; c. 4–20.

Further remarks can be highlighted:

- For the mixture D20-d16, regardless the percentage proportion, the macrotexture values and trends are close due to the small difference between the two radii.
- As the d/D ratio increases, a decreasing trend can be observed as a function of the incidence of fine (d variable) with respect to larger particles (D = 20 mm).
- In any case, within the percentage proportion at 75% of the particle size with diameter 20 mm, the macrotexture value is rater constant and close to 5 mm. In particular this aspect can be ascribed to the segregation phenomenon, which is strongly visible into the D20/d4 mixture, where the different dimensions of the particles are more accentuated (see Fig. 8).

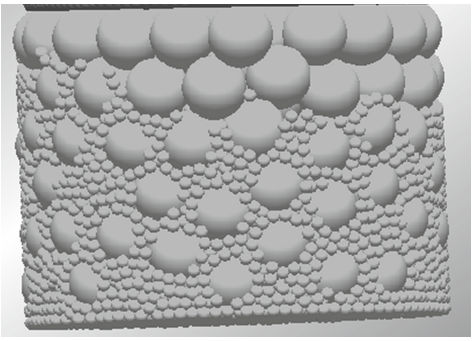

Fig. 8. Particular of the segregation phenomenon into the mixture D20/d4.

3.2 Void Content Diagram Representation of Macrotexture

In analogy with the model proposed for the representation of the voids content diagrams of two-component mixtures proposed by Furnas, the Macrotexture values of the mixes, at the fixed time of 10 s, have been arranged in the Fig. 9.

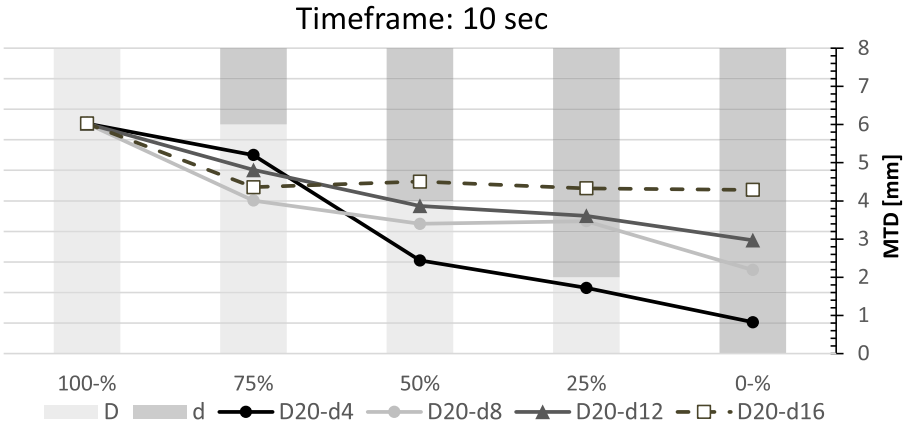

Fig. 9. Void content diagram of the macrotexture values representation.

Although the shape of the curves is different from the theoretical void ratio diagrams, even in the case of the representation of the macro texture, it can be seen that, for the same percentage, MTD values increase as the d/D ratio increases.

In particular, for each two-component mix, a decreasing trend can be seen as the diameter of the fine fraction decreases, with an increasingly accentuated slope. This concept is evident by observing the Table 3, where the summary of the regression data of each mix, has been reported.

Table 3. Summary of the regression data of the two-component analyzed mixtures.

Mixture code	d/D	Intercept	Angular coef. (Ac)	R^2
D20-D16	0.8	5.8547	−0.0201	0.65
D20-D12	0.6	6.1467	−0.0342	0.93
D20-D8	0.4	5.9527	−0.0385	0.87
D20-D4	0.2	6.3185	−0.0592	0.95

In the Fig. 10, a linear dependence can be found between the d/D ratio and the Angular coefficient (Ac) of the four analyzed mixtures. On the other hand, the intercept value, characterized with the mean of 6.07 and standard deviation of 0.21, can be considered as a constant.

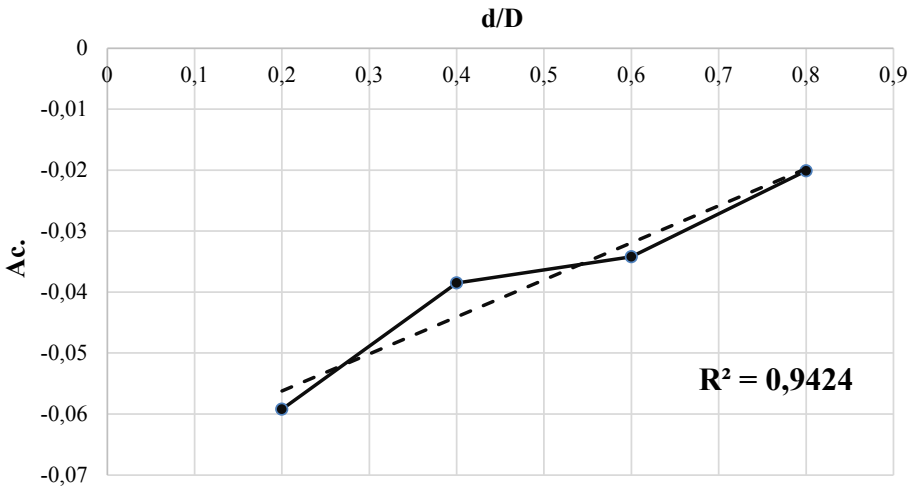

Fig. 10. Found Relationship between Angular coefficient (Ac) and d/D ratio.

From these premises, the extension of the voids predictive model of multi-component mix to macrotexture was analyzed. The proposed procedure is presented below.

4 The Power Diagram Representation for Macrotexture Prediction of Multi-component Systems

The proposed extension of the results obtained for the two-component mixture into the multi-component systems for the macrotexture prediction, has been reported in the following flowchart (Fig. 11).

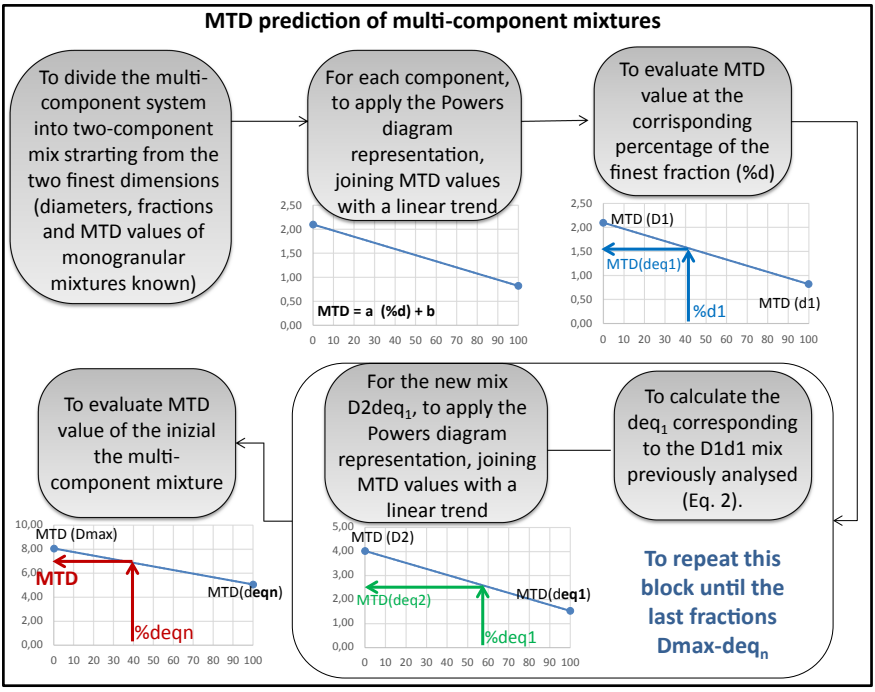

Fig. 11. Flowchart of the extension of the macrotexture evaluation from two-component to multi-component mixes.

In order to illustrate its applicability, an example has been provided below.

4.1 Example of the Proposed Method

The input data of the numerical example have been reported in the Table 4.

The first step consists into the evaluation of the incidence of the finest fraction (d) respect to the larger (D) considering the multi-component mix as a combination of three different two-component mixtures:

1. d4-D8;
2. Deq1-D12;
3. Deq2-D20.

Table 4. Input data of the numerical example.

N° fractions	Incidence [%]	Diameter [mm]	MTD monogranular [mm]
1	44	20	6.59
2	27	12	2.97
3	19	8	2.1
4	10	4	0.82

For each two-component mix, by means of the Eq. 2 the equivalent diameter corresponding to a monogranular mix have been evaluated. Then starting from the finest two-component mix (d4-D8), the Void Content diagram representation, joining the MTD values corresponding to the monogranular mixtures, has been performed and the same cascade procedure have been applied to the others sub-groups of two-component mixtures. The results have been summarized in the Table 5.

Table 5. Results of the multi-component mixtures

	Original incidence [%]	New incidence [%]	Diameter [mm]	Linear equation	MTD [mm]
d4	10	34.48	4		–
D8	19	65.52	8		–
Tot	29	100.00	–	$y = -0.0128x + 2.1$	1.66
D12	27	48.21	12		–
deq1	29	51.79	6.9		–
Tot	56	100.00	–	$y = -0.0131x + 2.97$	2.29
D20	44	44.00	20		–
deq2	56	56.00	10.0		–
Tot	100	100.00	–	$y = -0.043x + 6.59$	**4.18**

By way of example, the final Void Content diagram representation, used for the MTD evaluation of the multi-component mix, have been reported in the Fig. 12.

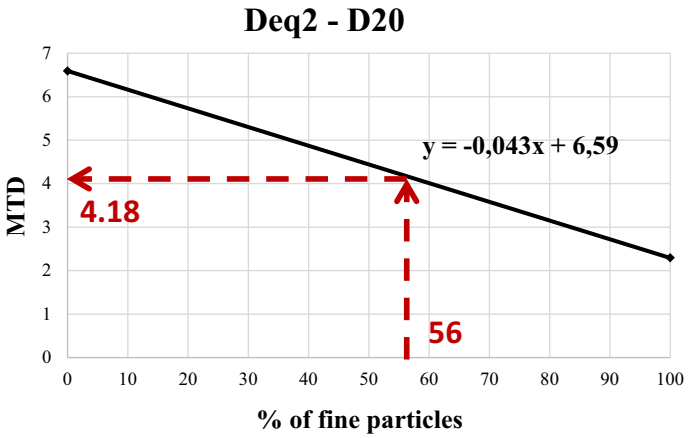

Fig. 12. Void Content diagram representation for the final MTD evaluation.

5 Conclusions

This paper presents intermediate findings obtained from the use of Void Content diagram representation for the description and prediction of the macrotexture. A simulation campaign has been performed with the aim to reproduce 20 different virtual gyratory compactor specimens with spherical particles. In particular four mixtures characterized by two different diameter dimensions (d-D) have been selected and, for each of them, five different percentage proportions have been identified.

An automated procedure for the construction of the virtual surface specimens and the related MTD values, has been proposed and the Void Content diagram representation has been applied to describe the macrotexture trend, depending on the d/D ratio.

According to the physical sense, the MTD values follow a decreasing trend as the fraction of fine particles increases respect to the coarse particles and this is further emphasized when the difference between the two diameters increasing (d/D ratio decreases). It can be due to the propensity of the fine fraction to occupy the interstitial voids of the coarse fraction.

Finally, a novel theoretical approach for the prediction of the macrotexture of multi-component mixtures, based on the Packing theory, has been proposed and a numerical example has been provided.

Intermediate results obtained so far, confirm that the DEM simulation can be an effective method for the macrotexture simulation also for two-component mixtures and that, although further analyses are needed, the Void Content diagram applied for the macrotexture description and prediction seems to show encouraging outcomes.

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