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Mesoscopic Generation of Random Concrete Structure Using Equivalent Space Method

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ABSTRACT

Concrete is a composite material with a wide variety of inhomogeneity. The mechanical behavior of concrete depends on the properties of its components. Mesoscopic model which treats concrete as a heterogeneous material consisting of coarse aggregates, mortar matrix with fine aggregates dissolved in it and Interfacial Transition Zone (ITZ) provides an effective approach to study how the properties of concrete components can affect its mechanical behavior. For such a study it is first necessary to generate a random concrete structure that resembles real concrete specimens. In this paper, an efficient simulation method for generating random concrete structure at mesolevel based on Monte Carlo random sampling principle is outlined and compared with two other most frequently used methods. A new method, the 'equivalent space method', appears to be more convenient for both low and high volume fraction specimens. In this method with each random selection of a value as the position of an aggregate particle with a definite size, more options for its position will be reached and examined. This leads to more realistic concrete models with less random numbers.

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1. Introduction

1.1. Concrete composite structure

Concrete is a complex inhomogeneous material in which particles, i.e. aggregates, are randomly dispersed in a matrix, i.e. cement paste. To this extent, the internal structure of concrete is heterogeneous, due to the existence of two phases, and it is complex due to the randomness of the aggregate particles.

Additionally, as concrete is mixed, more water surrounds the coarser aggregates. That is why the composite structure of cement in the vicinity of these aggregates seems more porous and fragile than the other areas. These weak areas are commonly known as interfacial transition zone (ITZ). Despite its insignificant thickness, about 10-50 μm [1–4], this area has an important effect on the concrete mechanical behavior. The effect of the properties of the ITZ on different concrete properties has been investigated by many researches. Abdelmoumen et al. [5] illustrate that the ITZ layer has a significant effect on better estimation of elastic properties of concrete composites. Also, He et al. [6] shown that the properties of this layer takes up a major position on tensile strength and fracture properties of concrete. Therefore, concrete may be considered as a three-phase system, consisting of a coarse aggregate, mortar matrix with fine aggregate dissolved in it, and the interfacial transition zone.

Modules of elasticity, thermal coefficient, and response to moisture changes, differ significantly over the aggregate and matrix phases. As concrete hardens, both heat of hydration and moisture losses occur simultaneously. As a result, due to the nonconformity of the properties between aggregate and matrix phases, cracks may develop. Usually, the ITZ represents the most potential location for such cracks, since it is the weakest link and located at the most critical place as far as stresses due to these effects are concerned. Therefore, cracks do exist in concrete prior to loading [7,8]. The existence of different phases causes material heterogeneities and the presence of interfacial transition zones has a high impact on the overall concrete mechanical behavior [9].

This is more than 30 years; concrete mechanical behavior is under different loading conditions has been investigated in various studies. While concrete homogenization is acceptable in engineering purposes, detailed information for mesoscale modeling heterogeneity of the material becomes profitable and even essential for situations where seriously spatial and stress and strain time variation is required, for instance in the study of local damages under the shock, blast or impact loads. Mesoscale models are also beneficial in studying mechanisms affecting the bulk behavior of material in different stress conditions [10], which shows the influence of the concrete behavior at the macro level. To consider these details, the concrete microstructure is needed to be simulated realistically and the concrete should be analyzed as a multi-phase composite material.

1.2 Modeling at various levels.

As mentioned, to scrutinize concrete behavior, it is advisable to properly consider the inherent inhomogeneity of its composite structure. Accordingly, Wittman [11] proposed three levels for modeling concrete, namely: macrolevel, mesolevel, and microlevel. At the macrolevel, concrete is considered as a homogeneous material while at mesolevel, it is assumed that concrete is an

amalgamation of a coarse aggregate, mortar matrix with fine aggregate dissolved in it, and ITZ. It is at this level that the geometry and distribution of aggregates come to the fore. At the microlevel, however, the mortar matrix of the previous level is regarded as a composite of fine aggregate and hardened cement paste with pores and micro-cracks embedded inside. The finite element mesoscale modeling development makes it possible to study the concrete bulk-scale behavior under different loading states and characterize the variation of the quantitative terms [10].

For such a mesoscopic study, it is first essential to generate the mesostructure of concrete material at this level, in which the configuration, size and distribution of the aggregate particles match actual concrete in the statistical evidence.

Various methods for simulating the distribution of aggregate particles in a way similar to the original concrete specimens have been introduced by different researchers. Wittmann et al. [12], Bazant et al. [13], Schlangen and van Mier [14] and Wang et al. [15], with a degree of sophistication, used the take-and-place method for generating random concrete structure for low particle volume fractions. In this method, aggregate particles are randomly taken from a grading curve and then placed within the concrete specimen in such a way that there is no overlap with the already placed particles.

De Schutter and Taerwe [16] used the divide-and-fill method for generating random concrete structures. In this simulation method, firstly, the concrete space should be separated into different parts. Then, each part should be filled with a grain particle that using a given grading curve and gravel content is reached.

For large volume portions of aggregates, Wriggers and Moftah [17] applied a method in which, whenever in the placing process, overlapping of a particle was revealed, the placed particle is moved to the minimum distance permitted between the particles to get rid of the overlapping problem. By keeping this distance fixed, the particle is then rotated randomly to find a suitable situation round the overlapping particle until all the placing requirements be satisfying.

Chen et al. [9] by presenting a new technique using digital image processing, captured the concrete section picture and produced the actual 3-phase concrete microstructure.

In the present study, in addition to a general review of the take-and-place method and the method proposed by Wriggers and Moftah [17], a new algorithm for generating mesoscopic geometry of concrete following a given grading curve has been suggested. In this algorithm, with each random selection of a value as the position of an aggregate particle with a definite size, more options for its position will be reached and examined. Using this algorithm will not only accelerate the process of generating random configuration of concrete at mesolevel but it will also open up an opportunity for generating specimens with higher volume fraction and comparable with real concrete specimens.

Finally, the efficiency of this method will be evaluated using building some specimens in comparison with the take-and-place method and the method suggested by Wriggers and Moftah [17].

2. Generating mesostructure of concrete

It is necessary to generate a random structure of the concrete specimen to evaluate it at mesolevel. Generating this random structure is based on the random distribution of aggregate and filling the space between them using mortar matrix. Since the generation of mortar matrix completely depends on how the aggregates are distributed, investigating this layer separately is not necessary.

This structure, which contains aggregates with random shape, size, and distribution, should as far as possible resemble the real concrete specimen in the statistical sense. For this purpose, the Monte Carlo's simulation method is used. This random method is used by sampling aggregates from a source whose distribution of their size is according to a certain grading curve. Then placing the aggregate particles will be done one by one into the concrete specimen such that there is no overlapping with placed particles [13].

As mentioned before, various methods have been proposed for accomplishing this and it is expected that two of most frequently used methods will be compared and contrasted with the method suggested in the current study.

Since aggregate particles have an indispensable role in generating the mesoscopic model, in what follows some general points regarding their shape and distribution will be provided and then the suggested method will be explained.

2.1. Aggregate phase generation

Aggregates constitute 60 to 80 percent of concrete volume and extremely affect its properties and the mix design of concrete specimens. Gravel and sand are among the most important particles used in concrete. Aggregates can be classified into two general classes: fine aggregates and coarse aggregates. Those particles with a diameter of larger than 4.75 mm are called coarse aggregates. Coarse aggregates account for 40 to 50 percent of the concrete volume in most concrete specimens. Moreover, in a general classification based on shape, aggregates can be divided into rounded shape and crushed shape. Many studies have so far attempted to discover the various features of aggregate shapes [12,15,18].

Wang et al. [15] and Wittmann et al. [12] generated gravel aggregates using the morphological law that was developed by Beddow and Meloy [19].

To simplify the process, other researchers, however, have used rounded or spherical aggregates [11–13]. In the current study, for the sake of simply assuming that the aggregates are rounded. Also, for classifying aggregates based on a specific criterion for size, smaller than 5 mm particles fall within the range of cement paste.

To generate simulation of a 2D random aggregate model compatible with the practical 3D cases, aggregate distributions transformation of 3D to 2D is a high important topic [20,21] but in this article, because the main goal is to presenting a new aggregate placing method and comparing with the other methods, this transformation has been neglected for simplicity.

2.1.1. Grading of aggregate

The grading curves used for determining particle size distribution of aggregates are often based on cumulative percentage passing through a series of standard sieves. Each grading curve can be demonstrated using a formula, table or graph. One of the best-known grading curves is proposed by Fuller which lies within the grading curves A32 and B32 of DIN 1045. Fuller curve can be illustrated by the following equation:

$$P(d) = 100 \left(\frac{d}{d_{\max}} \right)^\eta \quad (1)$$

Where $P(d)$ stands for the accumulative percentage passing through a sieve with the diameter d , d_{\max} is the maximum size of aggregate and η is a value between 0.45 and 0.7.

In a concrete mix, the total amount of coarse aggregate is usually given in terms of weight per unit volume of concrete. Therefore, the volume fraction of coarse aggregates can be obtained by dividing the weight of coarse aggregates per volume of concrete by the density of the aggregate. This ratio is about 0.4-0.5 for most concrete [15].

Due to the border effect, that no particle can come closer to the concrete surface than a distance equal to the particle radius, there is a smaller amount of aggregate near the concrete surface [15]. In case that the selected section for generating tow dimensional mesoscopic configuration, is placed at the proper distance to the surface of the concrete specimen, border effect can be neglected and the area ratio of aggregate is equal to the volume fraction.

If $P(d)$ is the cumulative percentage passing a sieve with aperture diameter d , Then the area of aggregate within each segment of the grading curve $[D_s, D_{s+1}]$, can be calculated as:

$$A_{\text{agg}}[D_s, D_{s+1}] = \frac{P(D_{s+1}) - P(D_s)}{P(D_{\max}) - P(D_{\min})} \times R_{\text{agg}} \times A_{\text{con}} \quad (2)$$

Where $A_{\text{agg}} [D_s, D_{s+1}]$ is the area of aggregate within the grading segment $[D_s, D_{s+1}]$, D_{\max} is the maximum size of aggregate, D_{\min} is the minimum size of coarse aggregate, R_{agg} is the area ratio of coarse aggregate and A_{con} is the area of concrete.

2.1.2. Taking process

Upon dividing the grading curve into several segments, the taking process begins with the grading segment containing the maximum size particles. The procedures for generating aggregates in each grading segment are as follows:

Step 1: Calculating the area of aggregate within each grading segment using formulae (3)

Step 2: Generating random numbers defining the size of the aggregate particle, assuming that the size D has a uniform distribution between D_s and D_{s+1} , through the following formula:

$$D = D_s + \eta \times (D_{s+1} - D_s) \quad (3)$$

In which η is a random number uniformly distributed between 0 and 1.

Step 3: Calculating the area of the generated aggregate and subtracting it from the area of the related segment.

Step 4: Repeating steps 2 and 3 until the area of aggregate left in each segment is less than $\pi D_s^2/4$. Since this area is not enough for generating another particle, the remaining area of aggregate to be generated is then transferred to the next grading segment.

Step 5: Repeating all the previous steps for the next grading segment, until the last particle of the smallest size has been generated.

2.1.3. Placing process

In the placing process, which starts with taking the maximum size particles, particles are placed into their proper positions into the concrete through satisfying a series of conditions. These conditions can be expressed in terms of the following two obvious terms: Firstly, the particles must be wholly within the boundary of the concrete area and secondly, there must be no overlapping between the placed particle with the already placed particles.

In addition to the aforementioned conditions, a third complementary condition can be considered separately: Each particle must be coated all around with a mortar film with the least thickness showing the distance of the particle boundaries to the concrete surface and the width of the gap between the particle and the ones in its adjacency.

For the minimum gap width between adjacent particles, Schlangen and van Mier [14] proposed the value of $0.1 \times \frac{(d_a+d_b)}{2}$ where d_a and d_b are the sizes of the two adjacent particles. On the same line of research, Wittmann et al. [22] have reached the conclusion that the thickness of the average mortar film changes as a response to the change in aggregate volume fraction, being smaller when the aggregate content is higher. Through visual inspection of cross-sections of hardened concrete, Wang et al. [15] have also focused on this topic. They proposed the value γd for the minimum thickness of the mortar film between a particle with size d and the boundaries of concrete, and the value γd for the minimum thickness of mortar film between two adjacent particles, where d is the size of the smaller particle and γ is the distribution factor whose value is dependent upon the aggregate volume fraction. The influence of satisfying each of these two conditions on the concrete homogeneity has been illustrated in Fig. 1. As can be seen in this figure, satisfying the condition proposed by Wang et al. [15] leads to a more homogeneous distribution of aggregate particles.

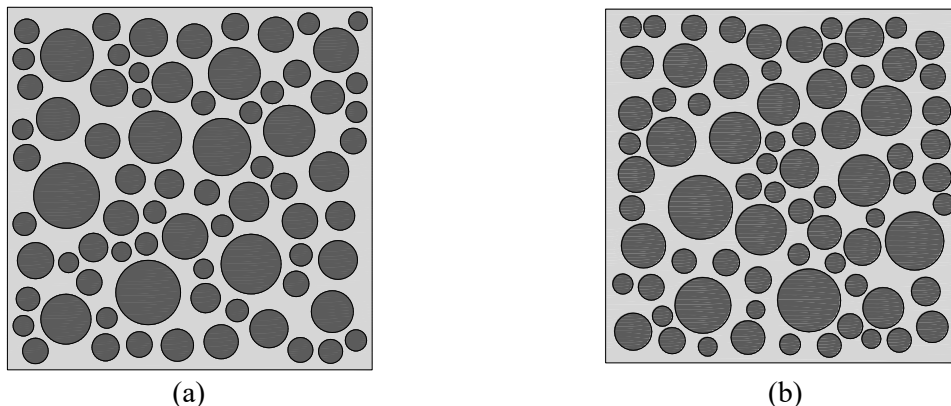


Fig. 1. The impact of satisfying the minimum gap width of a) Wang et al. [15] and b) Schlangen and van Mier [14] on the homogeneity of concrete.

The distribution factor γ has a significant influence on the spatial distribution of aggregate particles. That is, the larger value is attributed to γ , the more uniformity in spatial distribution of aggregate particles will be reached. Attributing a larger value to γ could possibly lead to difficulties in finding enough space to place particles. On the other hand, although a smaller value of γ would allow easier placing process, the distribution of the generated configuration would be less homogenous. At the outset of the placing process, the value of γ is determined according to the aggregate volume fraction; therefore, as an appropriate value, 0.3 can be attributed to γ in this process. If any difficulties during the placing process are encountered due to the lack of space, the value of γ can be reduced and the whole placing process restarted. Upon facing such difficulties, the process is iteratively done until the placement of all the aggregate particles in the concrete is accomplished.

A case in point at this juncture is that the feasibility of the third condition can be examined while checking the first two conditions. To do so, the size of the particles should be multiplied by $(1 + \gamma)$ while checking the first condition and the size of the particle to be placed within the concrete should be multiplied by the above factor while checking the second condition.

2.1.3.1. Equivalent space algorithm

The concrete section, whose configuration is to be randomly generated, may have a rectangular, circular or any other arbitrary shape. The scope of the present study, however, is limited to placing aggregate particles into rectangular-shaped sections.

Having selected the geometrical shape of the concrete section, placing the aggregate particles will be done according to the following procedures:

First, for every generated diameter in the taking process, an equal space to the concrete specimen should be duplicated. This equivalent space which is filled with aggregate particles with equal size completely conforms to the original concrete specimen in shape and dimension. Assuming a Cartesian coordinate system $X - Y$ with the origin O , the first aggregate with the coordinates X_0 and Y_0 on its center is placed in the equivalent space. The values X_0 and Y_0 are selected in a range that no space is left for placing another particle with the same size between the first aggregate and the axes that conform to the sides of the concrete specimen. Fig. 2 depicts the appropriate position for selecting the center of the first aggregate with a diameter d and Eq. (4) defines this position.

$$r + \gamma d \leq X_0 \leq 3r + 2\gamma d$$

$$r + \gamma d \leq Y_0 \leq 3r + 2\gamma d \quad (4)$$

$$\sqrt{(x - (r + \gamma d))^2 + (y - (r + \gamma d))^2} < 2r + \gamma d$$

From placing the first particle until filling the equivalent space, particles with the same size, satisfying the placing conditions, are successively placed within the equivalent space (Fig. 3). It goes without saying that as a result of the random position of the first aggregate, the position of the other aggregates will be random as well.

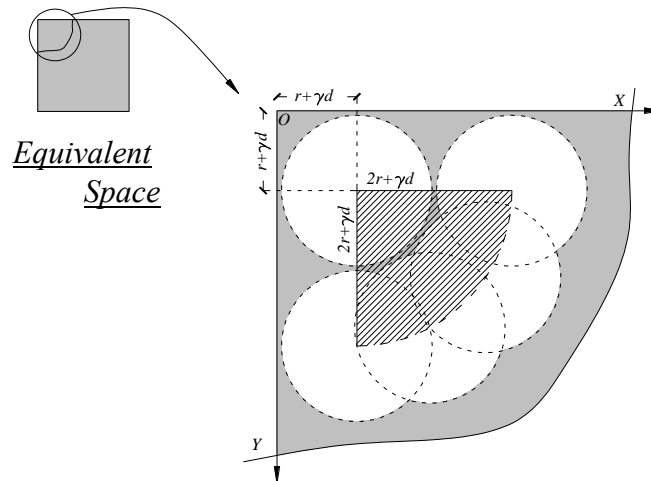


Fig. 2. Appropriate position for selecting the center of the first aggregate with a diameter d .

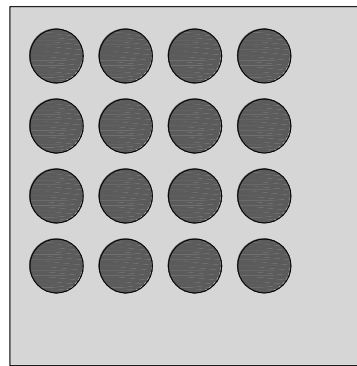


Fig. 3. Equivalent space, filled with the same size aggregates.

Having done all the aforementioned steps for all the particles resulting from the taking process, a required number of aggregates with different sizes are taken and placed within the original concrete specimen.

Here, initially, an equivalent space that is filled with the largest aggregate is selected and by generating a series of random values in the range with the maximum number of aggregates within the equivalent space, the desired number of aggregates with this size is taken and the rest is removed. Maintaining their location, the taken aggregates in this area are placed in the original specimen.

In the next step the equivalent space is generated by smaller size aggregates and after matching the boundaries of these spaces with boundaries of the original specimen, which contains the particles from the previous step, the aggregates which do not satisfy the placing conditions are cleared from equivalent space. Afterward, through generating a series of random numbers in the range with the maximum number of the remaining aggregate particles, a required number of aggregate particles is taken and the rest is cleared. The taken aggregate particles will be placed within the original specimen while maintaining their location. This process is iteratively done for the other aggregate particles until the placing of the smallest particle is accomplished. If during

the placing process adequate space for some aggregates of a size is not left, the equivalent space for this size is recreated by a random selection of a center for the first aggregate. Thereby through matching the boundaries of the equivalent space with the original specimen, the attempt for placing the remaining aggregates is resumed. The process is iteratively done until enough space for all the aggregate particles is provided. In case adequate space for placing aggregate particles within the concrete specimen should not be provided after repeating the aforementioned step, the next placing process would be restarted after reducing the value of γ .

Finally, the placing procedure of particles within the mesoscopic concrete specimen can be summarized as follows:

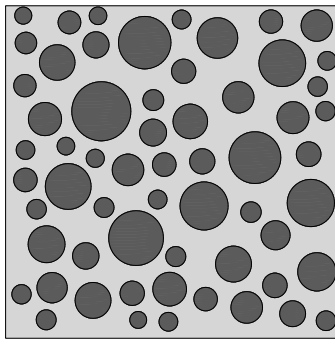
- Step 1: Generating an equivalent space for each size (diameter) through a random selection of a center for the first aggregate of that size in range defined by equation (4) and is shown in Fig 2.
- Step 2: Generate a virtual sample (specimen) and place the generated particle in the previous step and generate and place particles with similar size and minimum distance as shown in Fig. 3 and Checking whether all the placing conditions for the aggregates in each equivalent space are completely satisfied after matching the boundaries of this space with the boundaries of the original specimen.
- Step 3: A required number of aggregate particles (generated in Step 2) that satisfy the placing conditions should be chosen randomly and should be placed within the original specimen while maintaining their location.
- Step 4: Stopping the placing process and clearing all the previously placed particles should be done a particle does not satisfy the required conditions after repeating the third step (the number of repetitions is decided by the user). The aforementioned processes can then be restarted after reducing the value of γ .
- Step 5: Repeating all the steps described above from the largest size to smallest until all particles are successfully placed into the concrete specimen.

3. Results and discussion

To evaluate the efficiency of the suggested method, at this phase, it will be compared and contrasted with the take-and-place method and the method proposed by Wriggers and Moftah [17]. Since these three methods differ only in the hypotheses regarding the placing process, for a better comparison of their efficiency, for each volume fraction, at the beginning, aggregate particles are generated with a consideration of the principles governing the taking process. Then, the generated particles are placed within the specimen according to the criteria of each method.

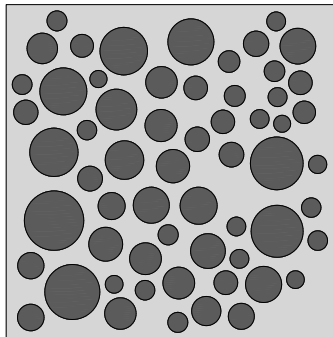
A comparison of the number of generated random numbers made to place all the aggregate particles within the concrete specimen has been done in Table 1. This table demonstrates all the information about the generated mesoscopic structure, such as coarse aggregates volume fraction, number of aggregate particles, γ and the number of generated random numbers made

for generating the mesoscopic geometry. All the concrete sections are 100×100 squares and in all cases, the minimum and maximum sizes of coarse aggregates are 5 and 19mm. Some examples of generated random configurations are presented in Fig. 4.



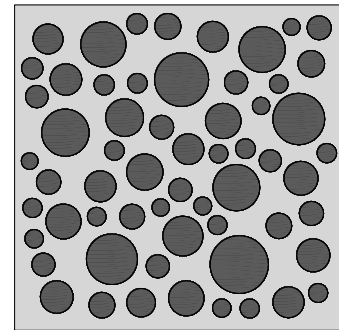
(a) Equivalent space method

$$\vartheta = 0.4, \gamma = 0.3$$



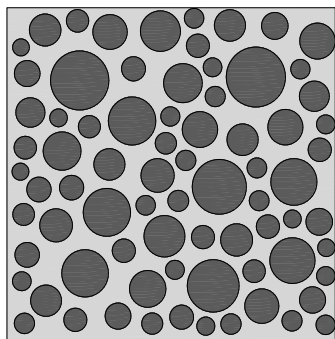
(b) The method proposed by Wriggers and Moftah [17].

$$\vartheta = 0.4, \gamma = 0.3$$



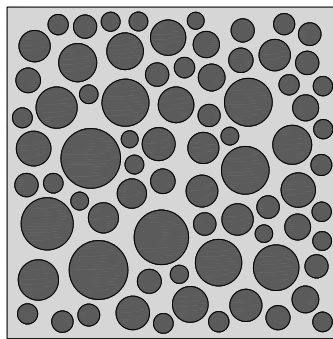
(c) Take and place method

$$\vartheta = 0.4, \gamma = 0.3$$



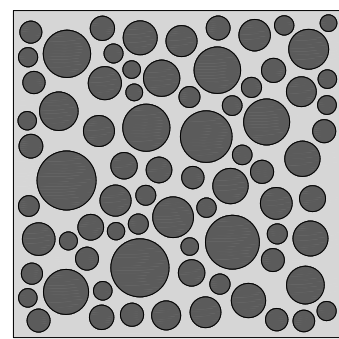
(a) Equivalent space method

$$\vartheta = 0.6, \gamma = 0.14$$



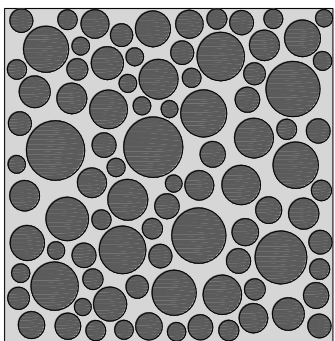
(b) The method proposed by Wriggers and Moftah [17].

$$\vartheta = 0.6, \gamma = 0.14$$



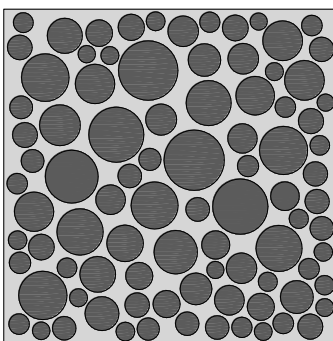
(c) Take and place method

$$\vartheta = 0.6, \gamma = 0.11$$



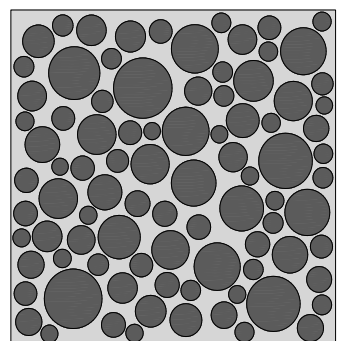
(a) Equivalent space method

$$\vartheta = 0.5, \gamma = 0.26$$



(b) The method proposed by Wriggers and Moftah [17].

$$\vartheta = 0.5, \gamma = 0.26$$



(c) Take and place method

$$\vartheta = 0.5, \gamma = 0.23$$

Fig. 4. Some examples of generated random configurations.

Table 1
Result comparison.

Volume Fraction	Method	Number of generated random numbers							NUM of AGG.	
$\vartheta = 0.4$	Equivalent space	66	64	62	61	61	60	60	60	60
	Wriggers and Moftah [17]	4130	3857	2796	3799	2637	3831	861	721	
	Take and place	4948	4230	2839	2567	1985	909	477	343	
$\vartheta = 0.5$	Equivalent space	----	----	----	5968	3211	1610	80	76	76
	Wriggers and Moftah [17]	----	----	----	----	71426	36193	6179	4367	
	Take and place	----	----	----	----	----	170968	5844	2106	
$\vartheta = 0.6$	Equivalent space	----	----	----	----	----	----	5177	1150	90
	Wriggers and Moftah [17]	----	----	----	----	----	----	82634	20128	
	Take and place	----	----	----	----	----	----	----	223690	
γ		0.3	0.29	0.28	0.27	0.26	0.23	0.14	0.11	

Investigating the Table 1 and the specimens generated above enables an understanding of the following points:

Take-and-place method:

1. This method has a relatively satisfactory function in generating specimens with a low volume ratio and the aggregate particles are distributed properly in the generated structure.
2. This method should be adopted for generating specimens with a high volume ratio, the aggregate particles would be placed with difficulty within the concrete specimen and the value of γ would be low.

The method suggested by Wriggers and Moftah [17].

1. Aggregates in High volume fraction specimens which are generated using this method can be placed within the concrete specimen with fewer attempts than the take-and-place method. Moreover, in these specimens, the aggregate particles would have a more appropriate distribution.
2. In lower volume fractions, however, due to this method's capitalizing on the translation-rotation algorithm, the distribution of the aggregate particles within the generated specimens would not be homogeneous.

The equivalent space method:

1. Using the method proposed in the current study, compared to the previous two methods, the aggregate particles can be placed within a concrete specimen with fewer attempts.

2. In specimens with an equal volume ratio, the proposed model can generate a mesoscopic structure with a higher γ . As γ can be considered a criterion for checking the level of specimen homogeneity, it is fair to claim that the aggregate particles in the specimens generated by this method would have a more homogeneous distribution.
3. In addition to the aforementioned points, the generated random configurations (Fig. 3) demonstrates that aggregate particles in the specimens generated via this placing algorithm can be placed appropriately within the specimens with various volume ratios.

4. Conclusion

In this paper, a new algorithm for generating random configuration of concrete at mesolevel is outlined and compared with two other methods. Applying the equivalent space method in high and low volume fractions would lead to generating specimens resembling the real concrete specimens. Using the algorithm proposed in the present study would lead to placing aggregate particles within concrete specimens with fewer attempts in comparison to the two most frequently used methods. As a result of comparing these methods, it becomes evident that in high volume fractions the placing algorithm does not have a significant influence on the homogeneity degree of a concrete section and it is the γ parameter which is the discriminating factor in this case. However, in low volume fractions, the effect of the placing algorithm on the degree of the generated structure homogeneity is significant. Here, the specimens generated via the model proposed in this study and the take-and-place method have a similar and appropriate condition. Whereas exploiting the method suggested by Wriggers and Mofteh [17] might not result in a homogeneous and appropriate distribution of aggregate particles.

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