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Rita Sassine, Etienne Malachanne, Eric Garcia-Diaz, Frédéric Dubois, Marc Vinches. Numerical simulation prediction for the elastic behavior of concrete taking into account its mesoscopic structure. ECCOMAS 2012 - European Congress on Computational Methods in Applied Sciences and Engineering, Sep 2012, Vienne, Austria. pp.5242-5255. hal-03260759

HAL Id: hal-03260759

<https://imt-mines-ales.hal.science/hal-03260759>

Submitted on 13 Jun 2024

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NUMERICAL SIMULATION PREDICTION FOR THE ELASTIC BEHAVIOR OF CONCRETE TAKING INTO ACCOUNT ITS MESOSCOPY

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Keywords: mesoscopic structure, concrete, mechanical properties, numerical simulation, finite element method.

Abstract. *For the purpose of studying the elastic behavior of concrete, a 3-D finite element model is used. A realistic method to represent concrete is adopted. At mesoscopic level, concrete is considered as a bi-phase material where coarse aggregates are dispersed in the mortar paste[1][1][1]. The coarse aggregates are represented as spheres and placed randomly in a cylindrical concrete specimen. The aggregate generation should respect the De Larrard model where the minimum paste thickness is taken into consideration. This generation should also respect a specific aggregate size distribution curve. A method to mesh the aggregates and the mortar separately is used. As a result, Different concrete specimens having different aggregate distribution and different aggregate content are generated. At that stage, a compression test is applied to each specimen in order to show the influence of the aggregate generation on the concrete properties. Analytical method and experimental results are used for the purpose of verifying the numerical approach. This model shows interesting results which can be used to predict the elastic behavior of concrete.*

I. INTRODUCTION:

Concrete is a composite material with a random microstructure [1]. The mechanical properties of concrete is directly affected by its content geometry and proportion as well as by the interface between the particles [2]. So, concrete is considered as a heterogeneous material composed of different constituents having different mechanical properties. Because of that, predicting the mechanical properties of concrete seems to be a complicated issue. Concrete is mainly characterized by its granular distribution content [3]. So, modeling concrete as a multiphase material is particularly interesting in order to see the impact of its granular composition on its mechanical properties as well as to visualize the behavior of concrete when changing its constituents properties.

Concrete internal structure is complicated to study especially because of the large difference of scale between its components[2]. At macro scale level, concrete is considered as a homogeneous material with equivalent properties. At mesoscale level, concrete is considered as a bi-phase material where coarse aggregates are surrounded by a mortar paste [4]. At this scale, the mortar is composed of cement and fine aggregates. It is important to mention that due to their large number and their small sizes, the fine aggregates are difficult to be represented in a concrete sample [5].

Numerical simulation methods are considered practical methods in order to visualize the mechanical behavior of concrete [6]. For this purpose, a numerical simulation based on the finite element method is adopted [7]. A software called LMGC90, developed by the university of UM2, is used to study the concrete response under different compression tests in three dimensions[8].

Different models exist for representing the skeleton of concrete. Some of them consider that there is no importance of the granular distribution curve and that the aggregates have random size and distribution[1]. In addition, some studies concern the prediction of the elastic properties of concrete using a combined image segmentation method where a 3D mortar image is taken by microtomography[9]. From the other hand, existing models give an importance to the structure of any concrete sample and consider that it has a direct influence on the mechanical properties of concrete. In our numerical model, the skeleton compressive model of De Larrard is adopted [10]. It introduces the idea of a maximum distance that should exists between adjacent aggregates, called maximum mortar thickness. So, the numerical aggregates are randomly generated in a specific concrete sample respecting a defined aggregate distribution curve [5]. Hence, The maximum mortar thickness is considered in the aggregate's generation process.

In order to validate our approach, some experimental results already done, are used [11]. The numerical Young's modulus of elasticity is found and compared with the experimental modulus. In addition, a comparison is made with different theoretical values that are calculated based on a homogenization approach [10].

II. EXPERIMENTAL WORK:

For the purpose of validating our numerical model, different experimental values issued from several research works are used [11]. Our study is based on a thesis that deals with lightweight concrete. For lightweight concrete, it is interesting to mention that the mortar has an important modulus of elasticity compared to the aggregate modulus and in contrary of the normal concrete [12]. The interesting approach is that the material properties are presented for different concrete mix as well as their appropriate compacity. So, concrete samples can be generated numerically respecting the experimental properties and specific aggregate distribution curves.

Different concrete samples having different compacities are studied. A mesoscopic biphasic approach where coarse aggregates are dispersed in the mortar paste is adopted. So, concrete is presented as a combination of aggregates and mortar having different material properties. Here below is a table presenting the Young's modulus of elasticity for different types of aggregates. In addition, the distribution of aggregates should respect a specific grading curve as shown in figure 1 where the minimum and maximum aggregate sizes are specified.

After identifying the aggregate properties as well as the mortar characteristics, compression tests are applied for the purpose of finding the equivalent Young's modulus of elasticity for concrete. The Young's modulus of elasticity for the mortar is taken to be equal to 35.4 GPa in all samples.

Aggregate type	E _{agg} (Gpa)
4/10 430 A	4,3
4/10 520 S	6,5
4/8 750 S	19,9

Table 1: Mechanical properties of aggregates [11].

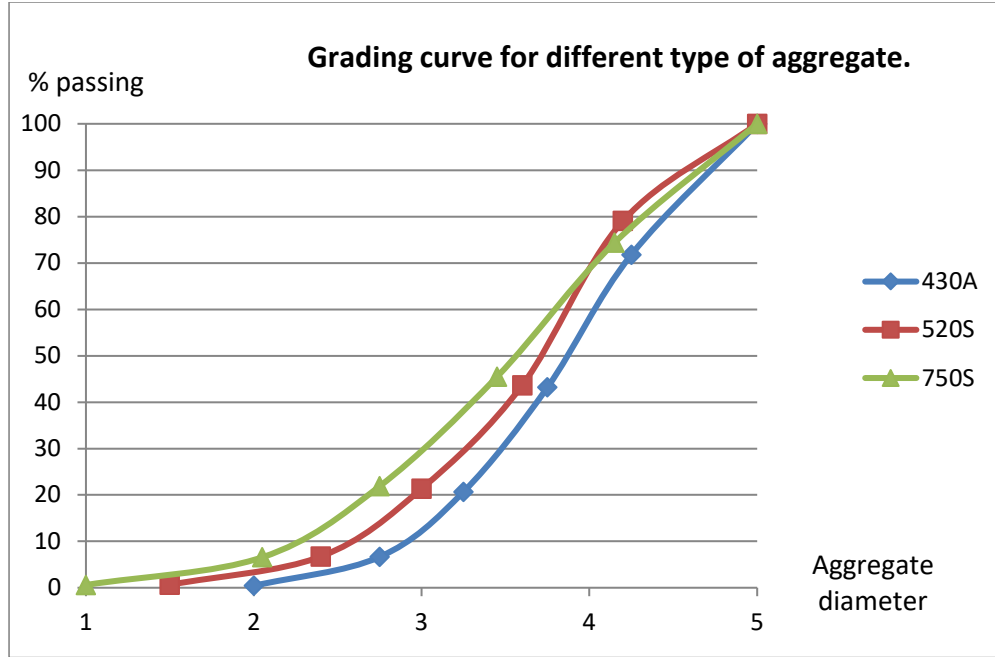


Figure 1: Grading curve for different types of aggregates.

III. GENERATION OF CONCRETE:

1. Compressive Model of De Larrard:

De Larrard introduces a model that represents concrete in a realistic way. He defines the principle of the compacity and the maximum compacity for any concrete sample [10]. The compacity represents the aggregate content in a concrete volume. It is defined as being the volume occupied by the aggregates in a unit volume of concrete. He specified also that a maximum distance should exist between adjacent aggregates for the purpose of having an optimal compacity for the concrete sample. He defines this distance as being the maximum mortar thickness.

The packing density (g) or the compacity of a granular mix is defined as being the volume of aggregates in a unit total volume of concrete. For any concrete mix, when aggregates are generated in a mortar paste, the objective is to combine grains in order to minimize the porosity.

The virtual packing density (g^*) or the virtual compacity is defined as the maximum packing density for a given mixture. So, it represents the maximum volume of aggregates that can be used for a specific volume of concrete. For rounded aggregates, the virtual compacity is calculated using the expression below:

$$g^* = 1 - 0.47 \left(\frac{d_{\min}}{d_{\max}} \right)^{0.22} \quad (1)$$

Where d_{\min} and d_{\max} are the minimum and maximum aggregate size.

The maximum mortar thickness (MMT) is defined as being the highest gap existing between two adjacent particles in a uniform dilatation process. This distance is defined by the equation below:

$$MMT = d_{\max} \left(\sqrt[3]{\frac{g^*}{g}} - 1 \right) \quad (2)$$

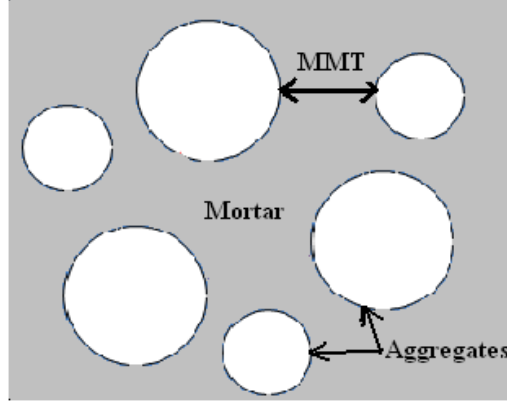


Figure 2: maximum mortar thickness (MMT).

2. Generation of concrete at mesoscale level:

Representing concrete at mesoscale level requires the generation of a numerical concrete with an aggregate structure, so a bi-phase material is generated [13]. For a mesoscopic approach, it is necessary to generate a random aggregate structure where the shape, size and distribution of the aggregates are close to reality. The generation mechanism is a three dimensional process where spherical aggregates are generated randomly in the concrete sample. This generation mechanism should respect the following requirements:

- The location of the aggregates is randomly chosen.
- The compacity or the aggregate content of the concrete sample is imposed.
- A specific aggregate distribution curve is respected as well as the minimum and maximum aggregate diameter.
- The aggregates are represented as spheres with random diameters ranging between a minimum and maximum imposed size.
- The maximum paste thickness is taken into account when aggregates are generated.

Once the aggregates are generated in the concrete sample, the mortar paste will fill the spaces between the particles.

3. Granular curve numerical simulation:

A numerical method is used to generate aggregates respecting a specific granular curve that is mainly depending on the spreading and the shape of the volume distribution. So, the objective is to find a simple function with a minimum number of parameters that is capable to draw curves similar to the classical granular curves [14]. For this purpose, a function β which represents the cumulative volume of aggregates is defined by the equation below:

$$\beta(dr, a, b) = \frac{1}{B(a, b)} \int_0^{dr} t^{a-1} (1-t)^{b-1} dt \quad \text{with } a > 0 \text{ and } b > 0 \quad (3)$$

Where a and b are the parameters that have influence on the shape of the granular curve.

$$dr = \frac{d - d_{\min}}{d_{\max} - d_{\min}} \quad \text{with } d \text{ the aggregate diameter } (0 \leq dr \leq 1) \quad (4)$$

$$B(a, b) = \Gamma(a)\Gamma(b)/\Gamma(a+b) \quad \text{with } \Gamma(x) = \int_0^\infty t^{x-1} e^{-t} dt \quad (5)$$

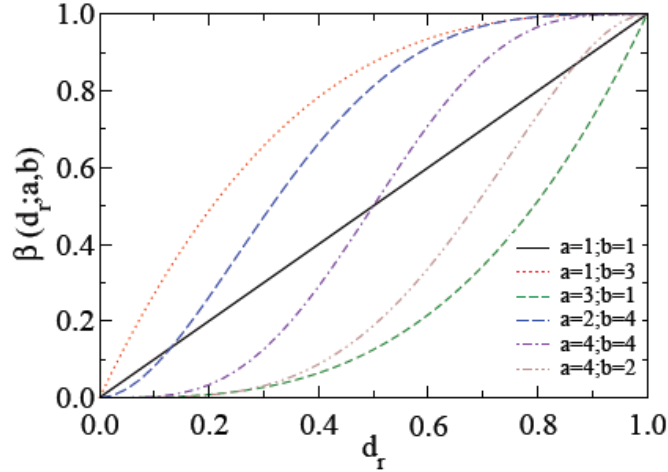


Figure 3: cumulative distribution curves with different values of a and b [14].

4. Algorithm

An algorithm is implemented using python language for the purpose of generating the aggregates. First, the aggregate dimensions are specified as well as the aggregate distribution curve that will be adopted in our calculations. The shape of the curve is defined using the function β as well as the parameters a and b . Once the desired curve is respected, the minimum and maximum aggregate diameters are specified. The software is capable to calculate the number of aggregates that should be generated in order to respect the desired curve. After specifying the aggregates dimensions, the generation of all particles is done. The aggregates are considered as spheres and deposited randomly in the concrete sample. The distance between the spheres should be less than the maximum paste thickness. The generation of the aggregates stops when an aggregate is generated near the boundary of the container.

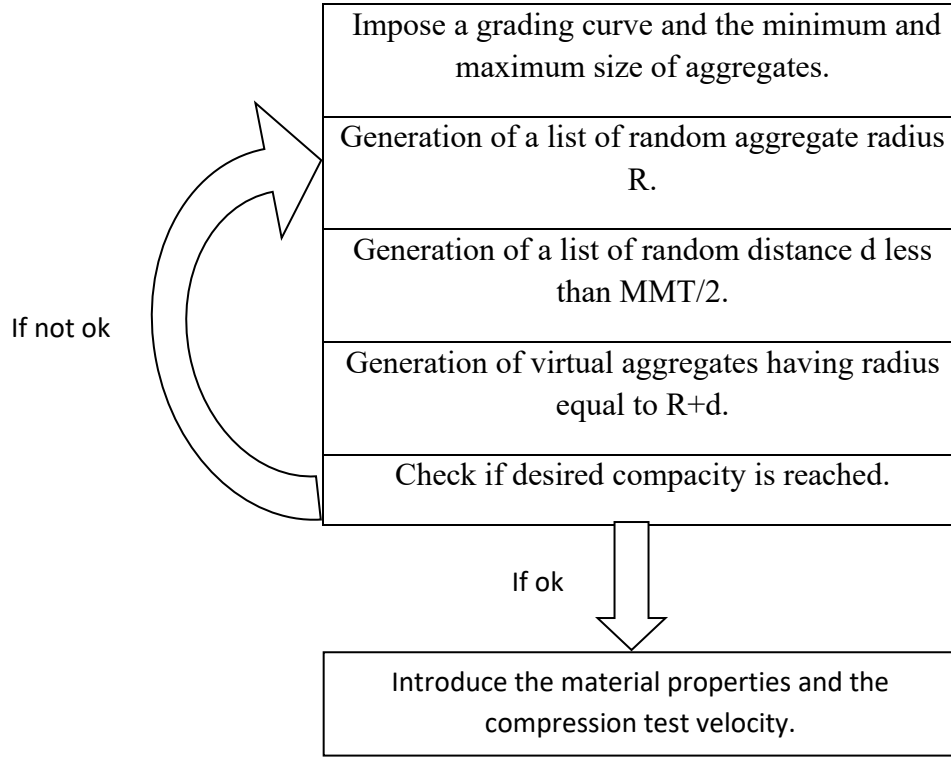


Figure 4: Random algorithm of aggregate generation.

III. CONCRETE HOMOGENISATION METHODS:

The principle of the homogenization models consists of representing a heterogeneous material as a homogeneous element having a unique response when applying a specific force[11]. Hence, the homogeneous behavior of concrete is identified at macroscopic level as a function of its properties at mesoscale level where the aggregates are differentiated from mortar. Different models of homogenization exist and are represented below.

1. The two sphere model of Hashin- Shtrikman:

In this model, concrete is considered as a bi-phase material, a phase of spherical particles dispersed in a continuous matrix, where all its components are perfectly bonded together [10]. It is considered as an isotropic composite having an elastic behavior with mechanical properties lying between two boundaries, called Hashin- Shtrikman bounds. For the bulk and shear moduli, the bounds are giving by the following equations:

$$K_{hi} = K_i + \frac{C_j}{\frac{1}{K_j - K_i} + \frac{3C_i}{3K_i + 4G_i}} \quad (5)$$

$$G_{hi} = G_i + \frac{C_j}{\frac{1}{G_j - G_i} + \frac{6(K_i + 2G_i)C_i}{5G_i(3K_i + 4G_i)}} \quad (6)$$

Where K_i , G_i , and i are the bulk modulus, the shear modulus and the concentration of phase i respectively. K_{hi} and K_{hj} (G_{hi} and G_{hj}) are the two bounds of the composite bulk (shear) modulus where i and j are the different phases with $c_i + c_j = 1$.

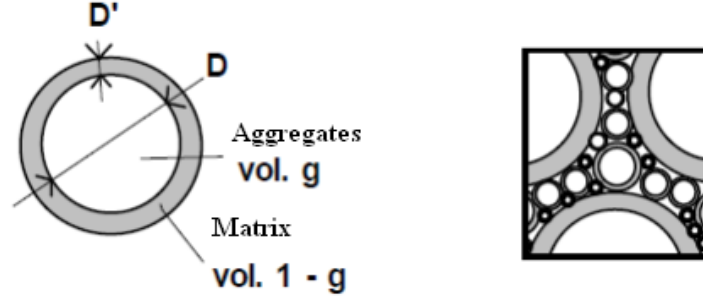


Figure 5: the two sphere model of Hashin et Shtrikman [10].

Hashin introduces the idea of a two-sphere basic cell for concrete homogenization. So, concrete is considered as a combination of spherical aggregates surrounded by a crust of matrix that completely fills the space as represented in figure 5. Replacing the equations above by their expressions in terms of elastic moduli with a coefficient of Poisson equal to 0.2 give us below expression modulus of elasticity is giving with the following expression:

$$E = \frac{(1+g)E_g + (1-g)E_m}{(1-g)E_g + (1+g)E_m} E_m \quad (7)$$

where E_g , E_m and E are the modulus of elasticity of aggregate, mortar and concrete respectively and g is the compacity of the mix. The same formulas as used in order to calculate the other boundary. It is sufficient to permute i and j in equations 5 and 6.

IV. NUMERICAL SIMULATION

LMGC90 is an open platform used for modeling interacting objects with different shapes and mechanical behavior in two or three dimensions [8]. It is considered as advanced research tool where new physical models and numerical strategies can be introduced. So, different objects with complex shapes can be represented in LMG90. This software is also capable to represent several models based on finite elements.

In our numerical model, after generating the aggregates and the mortar paste as described before, it is time to mesh the elements. For our case, the mesh is chosen to be tetrahedron. It is also important to mention that aggregates are meshed differently than mortar and the size of the mesh is not similar for both cases (figure 7). For the aggregates, the size of the mesh is considered proportional to the radius. So, aggregates having different size are meshed in a way to have the same number of elements. From the other hand, the size of the mesh of the mortar is considered to be constant for the entire sample.

Experimental results show that the interface zone for lightweight concrete doesn't exist or it is considered perfect [11]. For this purpose, our calculations are done for lightweight concrete and not normal concrete. So, the calculations are less complicated and no interface zone is considered between particles.

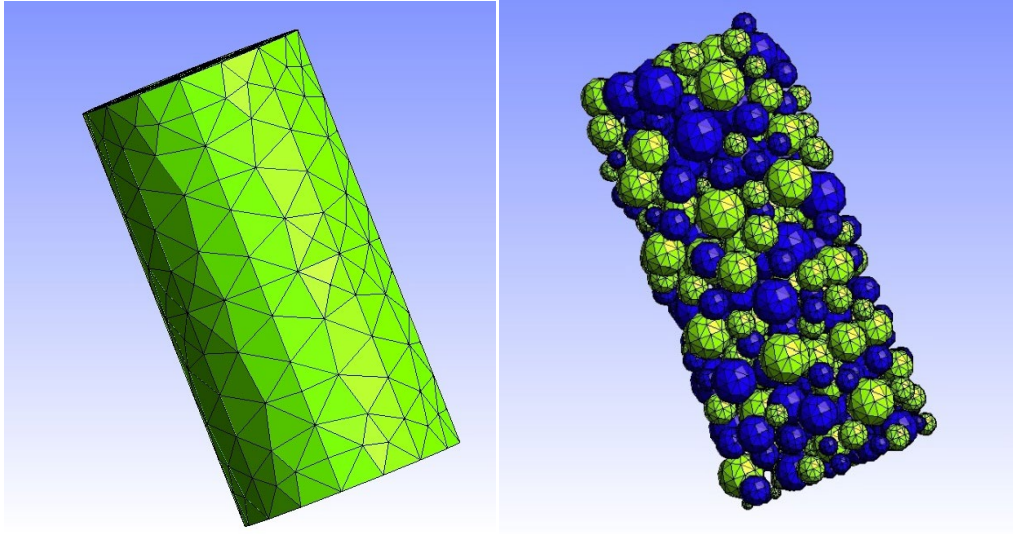


Figure 6: meshing of mortar and aggregates separately.

A main problem exists concerning the long time needed for running our calculations. In fact, the size of the mesh should be adequate to the size of the materials that have to be meshed, the aggregates in our case. Since the size of the generated aggregates is relatively small, the number of elements obtained after meshing the materials is important. As a result, the time needed for calculation is considered long. For this purpose, our objective is to find the size of the specimen in a way to have a realistic size of the mesh with an appropriate size of the specimen. After several tests, we find out that a concrete cylinder with a diameter of 40mm and a length of 80mm is suitable in our case. The size of the chosen mesh is sufficient and leads to accurate values. The diameter of the sample is higher than three times the diameter of the coarsest aggregate [15].

V. RESULTS:

Six different samples with three different aggregate types are studied for the purpose of validating our model. Here below are the properties of these samples where E_g and E_m are the Young's modulus of elasticity for the aggregates and the mortar respectively. g^* is the virtual

compacity for the different samples and g is the compacity adopted in the numerical simulation. Please note that a compacity of 12.5% is difficult to achieve in our calculations. Because of that a slightly higher compacity is adopted in order to find the equivalent numerical Young's modulus of elasticity for the desired samples. After generating the aggregate skeleton respecting the maximum mortar thickness and meshing the generated samples, a compression test is applied. The compression velocity is chosen to be equal to 2.10^{-5} m/sec and it is applied for 1 sec.

Compacity	Aggregate type	g	g^*	E_g (Gpa)	E_m (Gpa)
12,50%	430A	0,16	0,62	4,3	35,4
	520S	0,14	0,64	6,5	35,4
	750S	0,13	0,67	19,9	35,4
45,00%	430A	0,46	0,62	4,3	35,4
	520S	0,45	0,64	6,5	35,4
	750S	0,46	0,67	19,9	35,4

Table 2: Concrete properties for different samples [11].

The stress and strain distribution for the concrete samples is visualized using Paraview. So, by looking at their distribution, the stress and strain values can be deduced at any chosen point. The technique that is adopted for finding the equivalent Young's modulus of elasticity for any concrete sample consists of choosing points that belong to a specific chosen plan. So, a section is done at a certain height of the sample in order to make our calculations. After finding the Young's modulus of elasticity at each point on the section, the average value is calculated. Hence, the equivalent Young's modulus of elasticity for the desired section is found. The same procedure is done for several locations in the concrete sample. At the end, an equivalent Young's modulus of elasticity is found for the entire specimen.

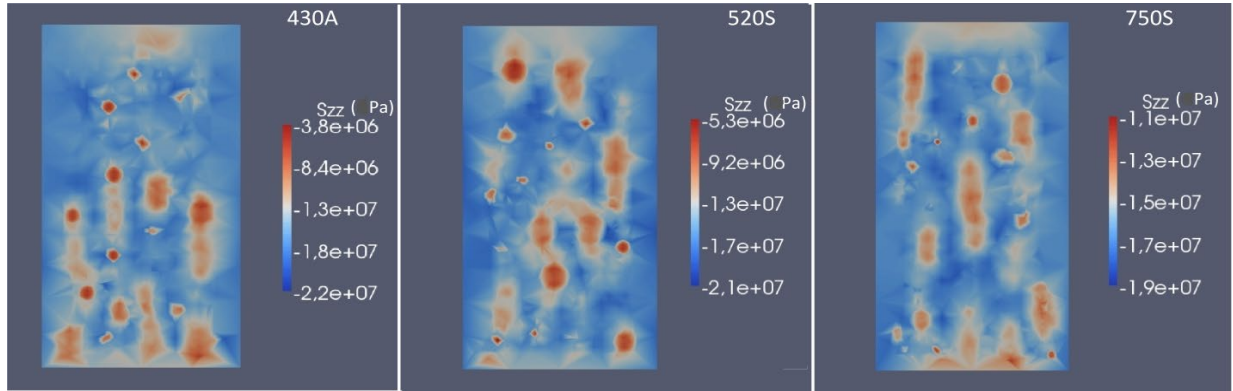


Figure 7: Stress distribution for concrete with a compacity of 12.5%

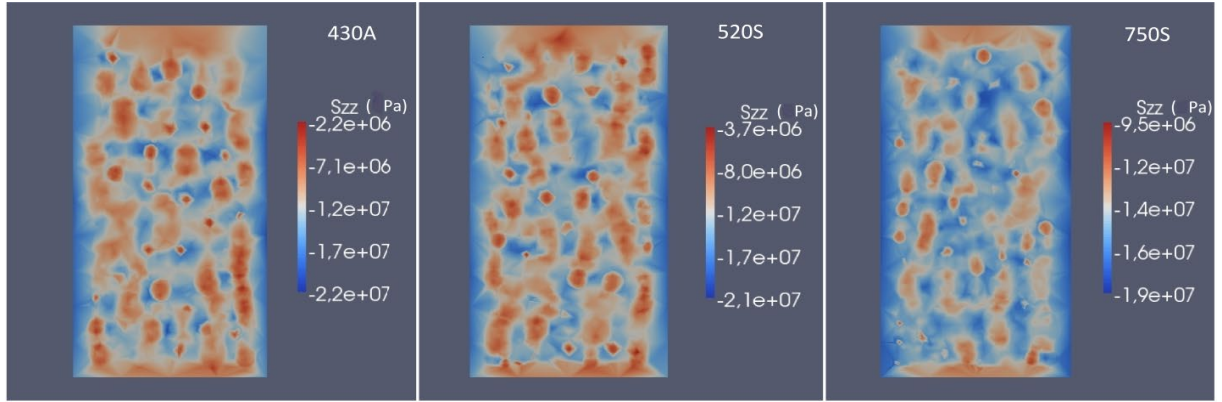


Figure 8: Stress distribution for concrete with a compacity of 45%

From figure 7 and 8, the difference of the stress distribution is obviously seen when the compacity of the concrete changes. For a compacity of 12.5%, we can clearly observe that the stress where the aggregates are present is less important than in the mortar. In addition, the difference in the stress distribution is also observed for the different concrete samples having different aggregate type. So, the difference of the stress distribution between aggregates and mortar for aggregates type 750S is less important than for the other samples. This aspect is justify by the fact that the Young's modulus of elasticity for this type of aggregates which is equal to 19.9 GPa is considered closer to the Young's modulus of mortar.

Here below are the equivalent Young's moduli of elasticity obtained for different concrete samples having the same mortar properties ($E_m = 35.4 \text{ MPa}$) and different aggregate content:

E_{agg} is the Young's modulus of elasticity for aggregates.

E_{exp} is the experimental equivalent Young's modulus of elasticity for concrete.

E_{num} is the numerical equivalent Young's modulus of elasticity for concrete.

E_{min} , E_{max} and E_{trisp} are the theoretical Young's modulus of elasticity for concrete obtained with the Hashin-Shtrikman approach and the trisphere model respectively.

The percentage mentioned on the top of each bar presents the percent difference of the mentioned values with the experimental results.

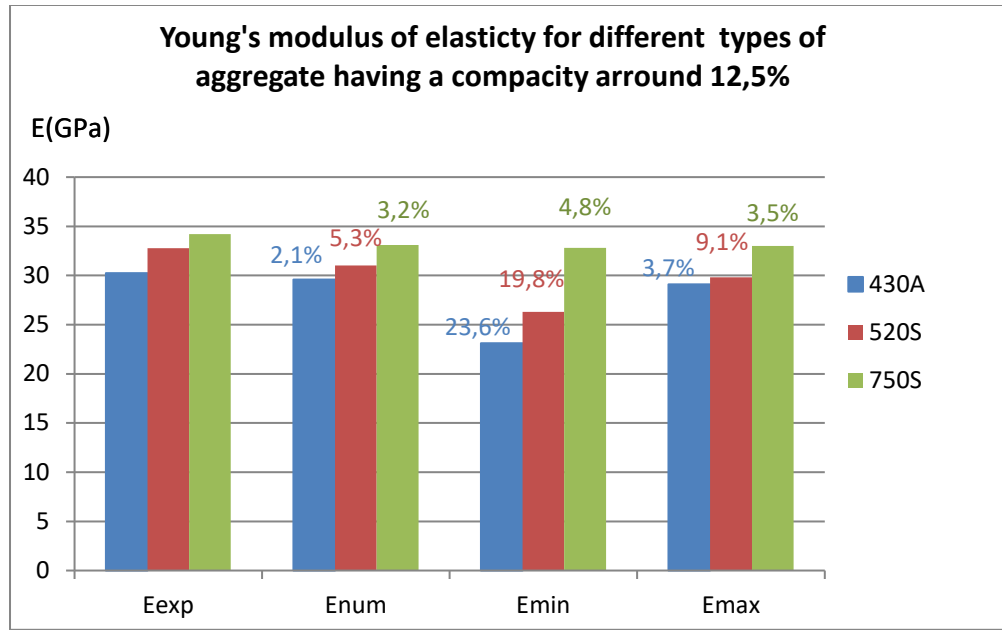


Figure 9: Equivalent Young's modulus of elasticity for different types of concrete samples having a compacity around 12.5%.

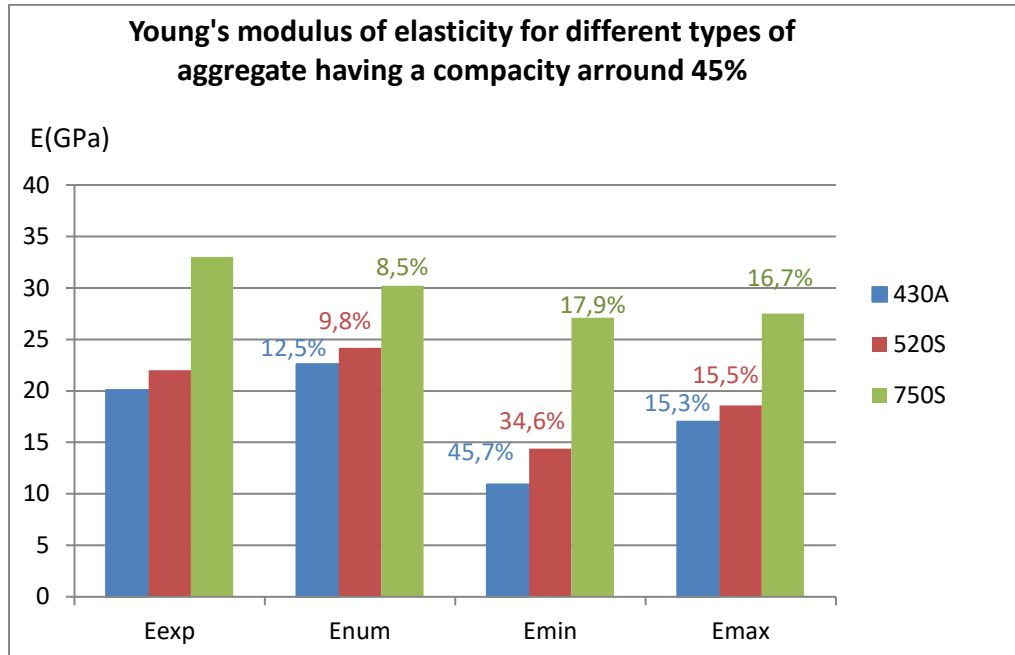


Figure 10: Equivalent Young's modulus of elasticity for different types of concrete samples having a compacity around 45%.

VI. DISCUSSION:

Our results show that the numerical Young's modulus of elasticity for the six samples is the closest to the experimental values. Comparing to the experiments, the numerical mechanical property of concrete presents a difference of less than 6% for a compacity of 12.5% and less than 13% with a compacity of 45%. These gaps seem to be negligible and acceptable in order to validate the numerical method. In addition, these results show that for a higher compacity, the percentage of difference between the numerical and experimental modulus is more important. So, by increasing the volume of aggregates in the concrete sample, the numerical modulus of Young shows significant difference with the experimental results. From the other hand, the Hashin-Shtrikman model gives mechanical properties that are not close enough to the experimental results. A difference between the analytical and the experimental Young's modulus that varies from 3.7% to 23.6% for a compacity of 12.5% and from 15.3% to 45.7% for a compacity of 45% , is observed. The homogenization model leads to different boundaries for the Young's modulus of elasticity. It is important to mention that for both cases, with different compacities, the experimental modulus of Young is closer to the maximal boundary than from the minimal boundary. So, we can deduce that the maximal boundary calculated with the Hashin-Shtrikman model leads to values that are close to the real Young's modulus of elasticity. From the other hand, a difference between the experimental values and the homogenization method shows that these approaches are not accurate enough in order to be adopted for calculating the equivalent Young's modulus of elasticity for concrete. As a result, the numerical approach seems to be the appropriate model that can be used to find the mechanical properties of concrete. Giving results that are close enough to the experimental work, our numerical model is considered more accurate than the homogenization approach.

From the other hand, we can link the fact that there is a more significant difference between the analytical results and the experimental values to the idea that there is no interface zone considered between the matrix and the inclusions in the numerical approach. The analytical models are used normally for the normal concrete and not for lightweight concrete. In addition, we can notice that a similar difference exists between the numerical and experimental results. So, when increasing the compacity the number of aggregates will increase. Hence, the margin between the experimental and the numerical moduli will also increase.

The compressive model of De Larrard for generating the numerical aggregates is considered to be a suitable model for generating concrete skeleton. Since the numerical results are close to the experimental values, we can conclude that the model of De Larrard represents concrete in a realistic way.

VII. CONCLUSION:

Our study shows that the compressive model of De Larrard seems to be a suitable model to represent concrete in a realistic way. So, by respecting a specific grading curve as well as the minimum and maximum diameters of aggregates that are present in the concrete sample, the results can be considered as correct. In addition, our 3D numerical model gives several results that are close to the experimental values which is not the case with the homogenization method. Hence, the numerical model is considered as an accurate approach to be adopted in order to visualize the elastic behavior of concrete at mesoscale level and to find its mechanical properties. At the end, it is interesting to find if the numerical approach we have already adopted for elastic zone is also valid for non elastic behavior of concrete. In addition, enlarging our research in order to find the influence of the grading curves used for the numerical approach on the mechanical properties of concrete, seems to be an important issue to study.

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