Multiscale modeling of the elastic moduli of lightweight aggregate concretes: numerical estimation and experimental validation

(Modelagem multiescala do módulo de elasticidade de concretos feitos com agregados leves: avaliação numérica e validação experimental)

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Resumo

Esse trabalho trata da simulação numérica do módulo de elasticidade efetivo de concretos leves através da técnica multiescala Homogeneização por Expansão Assintótica. A partir das propriedades elásticas do agregado e da argamassa empregados na composição do concreto, é possível calcular o tensor elástico homogeneizado do material resultante. O presente trabalho descreve o estudo numérico feito com concretos leves fabricados com a mesma argamassa e cinco tipos de agregados leves, com frações volumétricas variadas. O modelo adotado para representar as propriedades geométricas e mecânicas do concreto é caracterizado pela simplicidade. Comparações dos resultados numéricos com medições experimentais indicam a potencialidade da técnica multiescala empregada para a simulação do módulo de elasticidade de concretos.

Palavras-chave: Concreto, modelagem multiescala, propriedades efetivas.

Abstract

This study concerns the numerical simulation of effective elasticity modulus of lightweight concrete by means of Asymptotic Expansion Homogenization. Taking as input data the elastic properties of the aggregate and mortar employed in the concrete composition, it is possible to evaluate a homogenized elastic tensor for the resulting material. The present work deals with lightweight concretes made of the same mortar and five families of low density aggregates, with varying aggregate volumetric fractions. The multiscale model employed to represent the geometric and mechanical properties of the concrete is characterized by a great deal of simplicity. The validation of the adopted procedure consisted of comparisons of the numerical results with experimental measurements, showing good agreement.

Keywords: *Concrete, multiscale modeling, effective properties.*

1. Introduction

It is well known that the macroscopic behavior of heterogeneous materials may be strongly influenced by microstructural characteristics, mainly concerning durability aspects and aggressive environmental conditions, which lead to progressive degradation (Piasta et al., 1984; Rostasy et al., 1980; Saad et al., 1996, Farage et al., 2003). In these cases, it is convenient to take into account the microscale aspects in the modeling of heterogeneous systems, in order to adequately simulate the macroscale effects. However, the detailed representation of the microstructural interactions often results in extremely complex problems, which may even turn the solution impossible due to the great demand of computational effort. This fact justifies the application of numerical multiscale techniques to the estimation of effective or homogenized properties, whose values are similar to those obtained from experimental measurements (Murad et al., 2001; Murad & Moyne, 2002a, 2002b; Romkes & Oden, 2004; LNCC, 2005). This work employs *A*symptotic *E*xpansion *H*omogenization (AEH), a multiscale technique which is applied to periodic media for estimating the effective mechanical properties of concretes. The numerical simulations accomplished herein are based on the results of an experimental program developed by Ke et al. (2006a, 2006b) for the characterization of lightweight concretes with varied volumetric fractions of expanded clay. Firstly, this work presents the overall aspects of the AEH applied to linear elasticity problems. Then the experimental program used as validation for the applied numerical procedure is described. The numerical analysis and results are finally presented, as well as the comparison of the estimated homogenized properties to their experimental counterpart.

2. Asymptotic expansion homogenization

2.1. General aspects

AEH is based on the assumption that a heterogeneous medium may be represented by a homogeneous one since its microstructure is periodic or repetitive. The technique basically consists of studying the different scales of a material, extrapolating the results from inferior or heterogeneous scales in order to obtain global or homogenized properties (Sanchez-Palencia, 1980). When applying AEH, a very important aspect is the definition of the geometric characteristics of the periodic cell, which is the smallest microstructural volume capable of adequately representing the global constitutive behavior of the medium. Once the geometrical and physical properties of a cell are known, it is assumed that these properties are periodically repeated over the structure. In periodic structures with two scales, AEH consists of uncoupling those scales into a *microscale* and a *macroscale*. The general procedure for AEH applying the *F*inite *E*lements *M*ethod (FEM) comprises the following steps, as stated by Chung et al. (2001): (1) definition of a global body X in a coordinate system x_i, consisting of the structure without microstructural details, and a local body Y in a coordinate system y_i, consisting of one microstructure period; (2) meshing of X and Y in finite elements; (3) primary variable approximation by an asymptotic series in scale parameter $\in$, which relates the two coordinate systems x_i and y_i; (4) derivation of hierarchical equations, specific for the treated problem; (5) definition of a homogenized elastic tensor in the microscale Y; (6) resolution of the homogenized problem in the macroscale X. The homogenization deals with partial differential equations related to heterogeneous materials with periodical structure, considering the assumption that the amount of periodic cells tends to infinity. The scale parameter $\in$ relates the characteristic dimension of the period (or periodic cell) to the characteristic dimensions of the macroscopic dominium.

2.2 AEH applied to Linear Elasticity

According to Chung et al. (2001), by considering a material whose microstructure is composed of multiple phases, periodically distributed over the body (Sanchez-Palencia, 1980; Farage et al., 2005), the periodic elastic material properties are defined by the following relations:

$$D^{\in}_{ijkl} = D_{ijkl}\left(\frac{x}{\in}\right) \tag{1}$$

where $(\ )^{\in}$ denotes quantities related to the *actual* non-homogeneous medium and D_{ijkl} stands for the material property variations in the heterogeneous microstructure Y. The linear elasticity problem is described by the equilibrium equation (2), boundary conditions (equations 3 and 4), strain-displacement relation (equation 5) and constitutive relation (equation 6); where $\sigma_{ij}^{Î}$ is the ij term of the internal stress tensor and f_I is the body force in the dominium Ω; $u_i^{\in}$ is the displacement in direction i; n_j is the vector normal to the boundary Ω and F_i is the external force applied on the boundary and $\varepsilon_{ij}^{\in}$ is the ij term of the strain tensor. The displacements are approximated by an asymptotic series in $\in$, given by equation (7), where u_i^0 is the macroscopic displacement and u_i^1, u_i^2,.... stand for the periodic displacements in more refined scales. As the heterogeneous *actual* medium is represented by two coordinate systems (x and $y=x/\in$), the derivatives originally in $x^{\in}$ must be expanded in a chain rule given by equation (8). In order to obtain the uncoupled equations that describe the microscale and the macroscale problems, the displacement u_i is replaced by equation (7) in the set of equations (2) to (6). The basis of the approximation is the assumption of $\in$ tending to 0, indicating that the number of periodic cells tends to infinity and the actual non-homogeneous structure is then approximated by a homogeneous one. In order to validate such an approximation, the resulting coefficients of $\in$ with negative exponent must be identically nulls. That leads to the conclusion that the homogenized solution u^0 is constant over the microscopic scale (u^0 does not depend on y), as indicated by equation (9).

$$\frac{\partial \sigma_{ij}^{\in}}{\partial x_j^{\in}} + f_i = 0 \text{ em } \Omega \tag{2}$$

$$u_i^{\in} = 0 \text{ em } \partial_1\Omega \tag{3}$$

$$\sigma_i^{\in} n_j = F_i \text{ em } \partial_2\Omega \tag{4}$$

$$\varepsilon_{ij}\left(u^{\in}\right) = \frac{1}{2}\left(\frac{\partial u_i^{\in}}{\partial x_j^{\in}} + \frac{\partial u_j^{\in}}{\partial x_i^{\in}}\right) \tag{5}$$

$$\sigma_{ij}^{\in} = D_{ijkl}^{\in}\varepsilon_{kl}\left(u^{\in}\right) \tag{6}$$

$$u_i^{\in}\left(x^{\in}\right) = u_i^{(0)}(x,y) + \in u_i^{(1)}(x,y) + \in^2 u_i^{(2)}(x,y) + \ldots \tag{7}$$

$$\frac{\partial}{\partial x_i^{\in}} = \frac{\partial}{\partial x_i} + \frac{1}{\in}\frac{\partial}{\partial y_j} \tag{8}$$

$$\frac{\partial}{\partial y_j} D_{ijkl}\left(\frac{\partial u_k^0}{\partial y_l}\right) = 0 \tag{9}$$

Equation (10) relates u_i^1 to the homogenized term u_i^0 and represents the microscale problem:

$$-\frac{\partial}{\partial y_j} D_{ijkl}\frac{\partial u_k^{(1)}}{\partial y_l} = \frac{\partial}{\partial y_i} D_{ijkl}\frac{\partial u_k^{(0)}}{\partial x_l} \tag{10}$$

where u^0 is a known quantity and u^1 is the unknown. The variational formulation of the problem described by equation (10) is:

$$\int_Y D_{ijkl}\frac{\partial u_k^{(1)}}{\partial y_l}\frac{\partial \nu}{\partial y_k} dy = \frac{\partial u_k^{(0)}}{\partial x_l}\int_Y \frac{\partial D_{ijkl}}{\partial y_l} \nu \, dy \tag{11}$$

where ν is a weight function. In order to avoid the need of solving u_i^1 in the periodic cell for every variation of u_i^0, the solution of the variational problem (11) is given by (12):

$$u_i^{(1)} = \chi_i^{kl}\frac{\partial u_k^{(0)}}{\partial x_l} + \tilde{u}_i^{(1)}(x) \tag{12}$$

where $\tilde{u}_i^{(1)}(x)$ is an integration constant and χ_i^{kl} is the solution to the variational problem (13):

$$\int_Y Dijkl\frac{\partial \chi_k^{mn}}{\partial y_l}\frac{\partial \nu_i}{\partial y_j} dy = \int_Y \nu_j \frac{\partial D_{ijmn}}{\partial y_i} dy \;;\; \forall \nu_i \in V_Y \tag{13}$$

The function χ_i^{kl} is known as the elastic corrector or characteristic function (Chung et al., 2001), independent of u_i^0.

Once χ_i^{kl} is determined, it is possible to obtain the homogenized elastic property tensor D^h from equation (14):

$$D_{ijmn}^h = \frac{1}{|Y|}\int_Y D_{ijmn}\left[\delta_{im}\delta_{jn} + \frac{\partial \chi_i^{mn}}{\partial y_j}\right] dy \tag{14}$$

which employs the average operator given by equation (15):

$$\langle . \rangle = \frac{1}{|Y|}\int_Y (.) \, dy \tag{15}$$

where |Y| is the volume of the microscopic domain (periodic cell).

The evaluated homogenized tensor D^h relates the macroscopic stress to the macroscopic strain in the periodic cell (The reference (Sanchez-Palencia, 1980) brings the complete formulation of the AEH applied to linear elasticity problems).

2.2.1 General procedure for the numerical evaluation of the elastic tensor via AEH and the Finite Element Method

The general steps to the evaluation of the effective elastic properties of periodic heterogeneous media via AEH and FEM are:

1) Identification of the periodic cell.

2) Meshing of the periodic cell in finite elements.

3) Evaluation of the elastic corrector (χ) through equation (13), rewritten as follows:

$$\sum_Y [B]^T [D][B]|J|[\chi] = \sum_Y [B]^T [D]|J| \tag{16}$$

where $\sum_Y$ stands for the integration over the periodic cell's volume, [B] is the differential operator, J is the jacobian operator and [D] is the elastic tensor of the finite element's material.

4) Evaluation of the homogenized elastic tensor D_h through equation (14), rewritten as follows:

$$D_h = \sum_Y \frac{Ve}{Vt}[D]([I] + [B][\chi]) \tag{17}$$

where V_e is the finite element volume, V_t is the periodic cell volume and [I] is the identity tensor.

3. Experimental program

3.1 Materials and mixture proportions

The experimental study program regards the concrete as a biphasic material, composed of a mortar matrix and aggregates.

*L*ightweight *A*ggregate's (LA) characteristics and volume fraction vary from one concrete to another, while the composition of the mortar matrix remains identical. Concretes made of five different families of expanded clay were characterized. The physical properties of the employed aggregates are presented in Table (1). The saturated surface's dry specific gravity values range from 0.88 to 1.58. Water absorption at 24 hours is between 6 and 24%. The matrix is a Portland CEM I 52.5 cement mortar with fine sand 0/2 mm. For each aggregate type, the mortar mix proportioning is kept unchanged. The water/cement and sand/cement ratios are kept constant at 0.446 and 1.4 while the volume of lightweight aggregate varies. The volume fraction, defined as the coarse aggregate volume divided by the total concrete volume, was 12.5%, 25.0%, 37.5% and 45.0%. The LA's are used after a 48 hour immersion to avoid any change of the water-to-cement ratio due to water absorption by the aggregates during mixing. The aggregates are then drained for 20 minutes until their surface moisture becomes constant. This water availability for cement hydration is deduced from mixing water. A superplasticizer is used to obtain equivalent slump. The details of mix proportions for lightweight concrete (LWAC) made with the 0/4 650A expanded clay are shown in Table (2); for the other aggregate types, the proportioning is obtained by taking into account the respective specific gravity given in Table (1). It is assumed that all the aggregates have a Poisson ratio of 0.20, while their elastic moduli (E_a) are given in Table (3).

3.2 Experimental methods

The specific gravity and water absorption of the lightweight aggregate were tested according to EN1097-6 (AFNOR, 2006). Four 16x32 cm cylindrical specimens were cast for each volume fraction. During the first 24 hours, the specimens were left in the mold and then they were removed and cured in water for 27 days. Uniaxial compressive tests were carried out using a hydraulic 3000kN press with imposed stress rate. Axial displacements of the samples were measured in its median part during the test by three displacement transducers LVDT supported by aluminum rings in contact with the specimen. The samples underwent three loading-unloading cycles, from 0.5MPa to 1/3 of the ultimate load. The first cycle is accomplished in order to avoid measurements affected by plastic deformations. The Young's modulus is then determined from the slopes of the second and third cycles, according to the procedure recommended by Torrenti et al. (1999). The results of compressive strengths and Young's modulus are the averages of measures obtained for 3 specimens.

Table 1 - Physical properties of the employed lightweight aggregates.

Agg. Type	Gran. Size (mm)	Spec. gravity (SSD)	Spec. gravity (OD)	Water abs (%)	Bulk unit weight (AD)
0/4 650 A	0-4	1.22 kg/m^3	0.93 kg/m^3	24.2	600 kg/m^3
4/10 550 A	4-10	1.13 kg/m^3	0.92 kg/m^3	19.4	560 kg/m^3
4/10 430 A	4-10	0.88 kg/m^3	0.74 kg/m^3	14.2	455 kg/m^3
4/10 520 S	4-10	1.03 kg/m^3	0.90 kg/m^3	8.3	493 kg/m^3
4/10 470 S	4-8	1.71 kg/m^3	1.58 kg/m^3	6.7	877 kg/m^3

Table 2 - Mix proportions for the lightweight concrete made with the 0/4 650A aggregate.

%	Water (kg/m^3)	Cement (kg/m^3)	Sand (kg/m^3)	LA type	LA (SSD) (kg/m^3)
0	336	754	1055	-	0
12.5	294	660	923	0/4 650A	153
25	252	565	792	0/4 650A	306
37.5	210	471	660	0/4 650A	459
45	185	414	580	0/4 650A	550

The 4th specimen is used to measure the concrete density after oven drying, according to EN12390-7 (AFNOR, 2006), and to determine a segregation index ($I_s=\rho_{top}/\rho_{bottom}$). The level of LWAC's segregation is estimated as the ratio of hardened densities of the upper to the lower part of a concrete cylinder. A possible segregation of LWAC then leads to a reduced density of the upper section of the specimen due to the tendency of the aggregates to float in the denser matrix. To obtain a sufficiently accurate index, concrete cylinder sections with 8 cm are sawn. Segregation problems are sometimes encountered at the lowest volume fractions with the lightest aggregates. Specimens with a segregation index lower than 0.98 are re-cast under better vibration control. The elastic properties of the employed mortar are E_m=28.58 GPa and ν =0.2. The measured elastic moduli for the tested concretes (E_c) are listed in Table (3).

4. Numerical evaluation of the effective elastic tensor

The AEH formulation for linear elasticity problems described in section 2.2 was implemented in the integrated technical computing environment Matlab© (Mathworks, 2009). The current version of the program (HEA2D) evaluates the effective or homogenized elastic tensor of two-dimensional cells via FEM (Farage et al., 2005; 2006), and was employed to evaluate the elastic properties of the concretes characterized in the experimental program presented in Section 3. The main purpose of this application is to verify the ability of the studied multiscale technique to determine the Young's modulus of concretes based on the following main assumptions: (a) the concrete is represented as a biphasic medium, composed of mortar and aggregate, both considered as isotropic; and (b) the heterogeneous microstructure is modeled by plane periodic square cells. The aggregate volumetric fraction in each concrete is represented in the cell by inclusions: the ratio between the inclusions' area and the cell's total area equals the aggregate proportion in the mixture. In order to verify the influence of the inclusion's geometry on the homogenized result, three simple geometric forms were adopted to model the medium. The typical aspects of the adopted periodic media and cells are shown in Figure (1), where the mortar is represented in white and the aggregates in black. The adoption of symmetric cells composed of isotropic phases leads to an isotropic homogenized tensor, described by the general formula (18):

$$D_h = \frac{E_h}{\left(1-\nu^2\right)}\begin{bmatrix} 1 & \nu & 0 \\ \nu & 1 & 0 \\ 0 & 0 & \frac{\left(1-\nu\right)}{2} \end{bmatrix} \quad (18)$$

Table 3 - Experimental and numeric data and results.

n	E_a (GPa)	f (%)	E_c (GPa)	E_{h1} (GPa)	E_{h2} (GPa)	E_{h3} (GPa)	e_1 (%)	e_2 (%)	e_3 (%)
1	6.47	12.5	23.54	23.79	23.81	23.49	1.08	1.16	0.20
2		25.0	20.67	20.16	20.18	19.34	2.45	2.33	6.39
3		37.5	16.74	16.93	17.20	15.96	1.13	2.70	4.66
4		45.0	15.67	15.45	15.61	14.24	1.39	0.40	9.09
5	7.5	12.5	24.90	24.17	24.19	23.92	2.94	2.84	3.95
6		25.0	21.39	20.74	20.78	20.05	3.03	2.88	6.25
7		37.5	17.29	17.67	17.92	16.86	2.15	3.64	2.52
8		45.0	15.70	16.25	16.39	15.21	3.48	4.43	3.10
9	8.03	12.5	26.16	24.35	24.38	24.12	6.90	6.80	7.77
10		25.0	21.68	21.03	21.07	20.40	2.98	2.82	5.90
11		37.5	17.90	18.03	18.29	17.30	0.75	2.16	3.36
12		45.0	16.61	16.65	16.79	15.69	0.24	1.11	5.50
13	10.23	12.5	25.14	25.08	24.90	22.17	0.34	0.23	0.94
14		25.0	22.42	22.17	22.20	21.73	1.12	0.95	3.08
15		37.5	19.43	19.49	19.72	19.01	0.33	1.52	2.16
16		45.0	18.29	18.24	18.37	17.57	0.25	0.45	3.92
17	20.23	12.5	27.37	27.35	27.35	27.33	0.08	0.06	0.14
18		25.0	26.26	26.19	26.20	26.13	0.28	0.25	0.48
19		37.5	25.28	25.01	24.11	25.00	1.07	0.69	1.09
20		45.0	24.32	24.43	24.47	24.36	0.44	0.62	0.14

f(%) is the aggregate volumetric fraction; E_a is the aggregate's Young's modulus; E_{ai} is the numeric homogenized modulus; e_i is the approximation error (Equation 19); subscripts $(.)_1$, $(.)_2$ and $(.)_3$ stand for cell types a, b and c respectively.

where D_h is the effective elastic tensor; n is the effective Poisson ratio and E_h is the homogenized Young's modulus for the composite material. The proposed geometric model was applied to the numerical estimation of the elastic tensors of the lightweight concretes characterized in the experimental program. As stated earlier, the concrete herein is considered as a biphasic medium, and the input data for the HEA2D program are the Young's Modulus (E_α) and the Poisson ratio (ν_α) of each component a: mortar and aggregate. The values adopted in this work were obtained from the described experimental program (see Section 3 and Table (3)). The HEA2D program gives as output the homogenized tensor D_h, from which the numeric modulus E_h may be evaluated. The typical aspects of the finite element meshes employed in the present study are shown in Figure (2), generated via the mesh generator Gmsh (Geuzane, 2008).

4.1 Comparison between the numeric and the experimental results

In order to analyze the numerical errors obtained from the three tested cells, the approximation errors were evaluated by Equation (19):

$$e_i = \left|\frac{E_c - E_{hi}}{E_c}\right| 100\% \qquad (19)$$

where E_c is the experimental Young's modulus of the tested concretes obtained from the experimental program; E_{hi} is the numeric homogenized Young's modulus and $(\ )_i$ identifies the cell type indicated in Figure (2) (where 1 stands for cell a, 2 for cell b and 3 for cell c). Information concerning the FE meshes employed to model concretes with varying aggregate volumetric fractions (f(%)) are listed in Table (4). As one can notice in Figure (3), the influence of the LA's f*(%)* on the E_c values is adequately represented by the evaluations accomplished with all 3 periodic cells. The errors e_i indicate that cells a and b lead to very similar values for E_h , denoting that these geometric forms are equivalent to representing the aggregates in the medium. Most of the

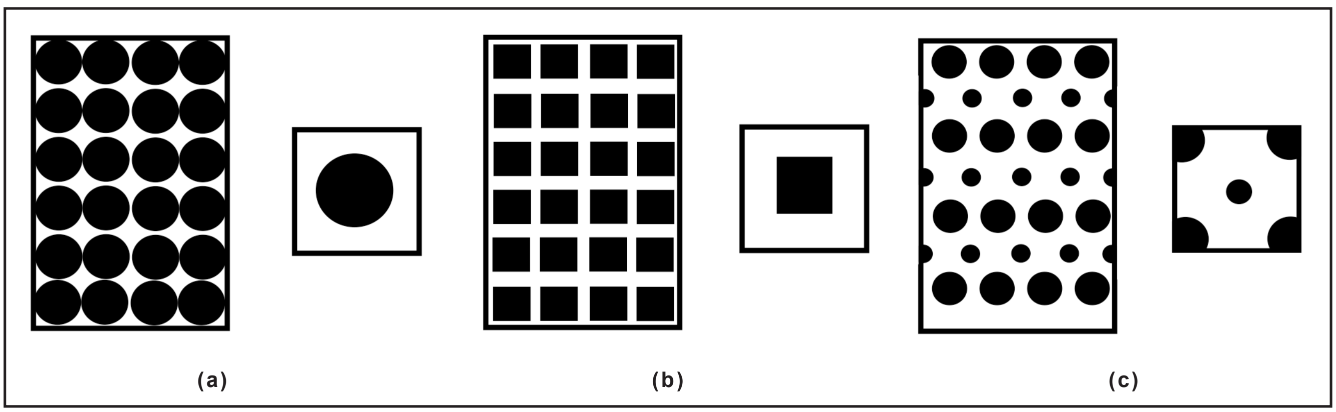

Figure 1 - Adopted geometric models for the periodic media and cells.

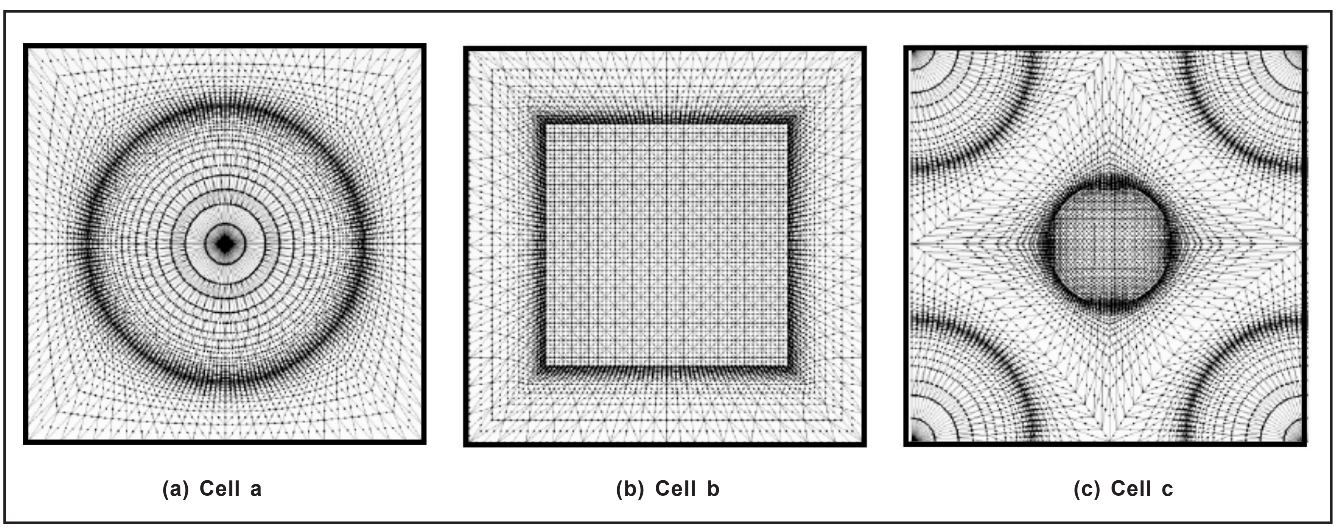

Figure 2 - Typical aspects of the adopted finite element meshes.

Table 4 - Meshes data.

f(%)	12.5%			25.0%			37.5%			45.0%		
Cell type	a	b	c	a	b	c	a	b	c	a	b	c
Nodes	8353	8161	8457	8353	8271	8509	8353	8177	8481	8353	8041	8509
Elements	4128	4032	4144	4128	4056	4182	4128	4032	4176	4128	3960	4182

evaluated errors e_1 and e_2 are less than 3%, except for one mixture for which the experimental value is rather more elevated than the expected (line 9 in Table (3)), which probably results from some experimental problem. Results obtained from cell c are rather different from the others, mainly for concretes with lower f(%). Such differences might indicate that the inclusion distribution in the periodic cell affects the evaluation of E_h. On the other hand, for the concretes made of aggregates with E_a=20,20GPa, there are no significant differences amongst the values obtained from the 3 cells, since the errors e_i are less than 1%. This fact might indicate that the homogenization is more effective for lower E_m/E_a ratios, but the authors believe that it is due to the FE meshes, whose refinement, mainly in the interface regions, do affect the approximations.

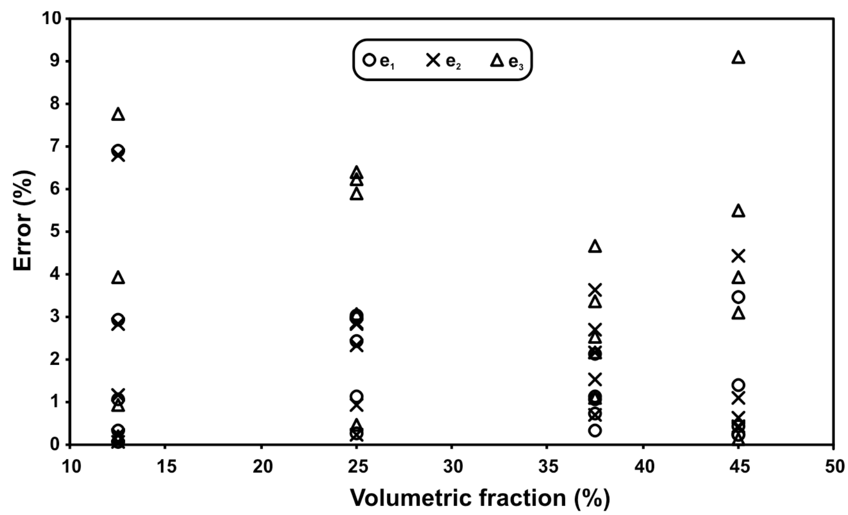

Figure 3 - Approximation errors e_i, given by equation (19), related to the three periodic cells.

5. Conclusions

Despite a number of simplifying hypotheses adopted to model the geometric and mechanical characteristics of the heterogeneous medium in study, the numeric results are similar to the experimental measurements taken as reference. The influence of the geometric distribution of the inclusions adopted to represent the aggregates in the periodic cell needs to be further analyzed, as herein the discrepancies observed among the numeric results obtained from three different geometries seem to have been more influenced by aspects related to the finite element meshes. The obtained results encourage the application of AEH to simulate more complex problems.

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