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HOMOGENEIZAÇÃO TÉRMICA DO CONCRETO LEVE UTILIZANDO MODELOS MICROMECÂNICOS DE CAMPOS MÉDIOS

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THERMAL HOMOGENIZATION OF LIGHTWEIGHT CONCRETE USING MEAN-FIELD MICROMECHANICAL MODELS

Resumo
Os modelos micromecânicos de campos médios são amplamente utilizados para a homogeneização de materiais heterogêneos com inclusões randômicas. O avanço da teoria da inclusão equivalente permitiu a determinação das propriedades físicas efetivas para diversos materiais compósitos. Com as propriedades de suas fases e as equações dos modelos propostos, pode-se realizar a homogeneização para a verificação com resultados experimentais. Este trabalho demonstra a obtenção das propriedades térmicas para aplicação na construção do concreto leve. Verifica-se que, com uma boa caracterização experimental das fases, é possível dispor de resultados analíticos que possibilitam um procedimento de escolha do percentual de inclusões no concreto, considerando a massa específica requerida e o desempenho térmico do material.
Palavras-chave: Micromecânica, Homogeneização, Concreto.

Abstract

Mean-field micromechanical models are widely used for the homogenization of heterogeneous materials with random inclusions. The advance of the theory of equivalent inclusion allowed the determination of the effective physical properties for several composite materials. With the properties of its phases and the equations of the proposed models, it is possible to carry out the homogenization for verification with experimental results. This work demonstrates the obtainment of thermal properties for application in the construction of lightweight concrete. It is verified that, with a good experimental characterization of the phases, it is possible to have analytical results that enable a procedure to choose the percentage of inclusions in the concrete, considering the required specific mass and the thermal performance of the material.
Keywords: Micromechanics, Homogenization, Concrete.

1 Introduction

The use of micromechanical models to predict the behavior of various engineering materials has grown over the years. The microstructure of these materials is complex, and somewhat random. For practical purposes, it should be considered that the properties of these materials are calculated based on the determination of a representative volume element (RVE).

For the homogenization of heterogeneous materials, the stress and strain fields are defined in terms of homogeneous boundary conditions, having as fundamental pillar the mean-stress and mean-strain theorems, in which the basic equations of micromechanics were developed. Thus, the estimation of the effective elastic properties of heterogeneous materials is one of the objectives of micromechanical analyzes based on mean-field theorems.

In this context, applications for the analysis of composite, cellular, porous and periodic materials stand out. The development and improvement of different models is still an area of study that receives relevant contributions for the design and evolution of new materials with structural applications, for example.

In the civil construction industry, concrete is the most consumed material in the most diverse applications. In this way, the demand for its understanding in terms of microstructure is explicit. Recent advances demonstrate that the micromechanical approach for determining the effective thermal properties for concrete is a topic of interest to the scientific community, as in (She, Zhao, Cai, Jiang, & Cao, 2018), (Sayadi, Tapia, Neitzert, & Clifton, 2016), (Xu, et al., 2016), (Wei, Yiqiang, Yunsheng, & Jones, 2013).

However, concrete is a composite material that has unique characteristics, which make difficult and/or require robust experimental analysis for model calibration. In this work, it is proposed to evaluate the construction and thermal and thermoelastic modeling of concrete with lightweight aggregates, evaluating the percentage of error in the use of micromechanical models in comparison with the experimental results obtained in the literature. Furthermore, it compares the different modeling strategies with parameter variations that influence the thermal behavior of the composite.

2 Preliminary Considerations on Homogenization of Composites

The homogenization of composites can be understood as a correlation of physical properties, presented in Table 1. Withers (Withers & J., 2000) presents a simple governing equation, in which the field of variables can be written in generic form (Equation 1):

$$\Psi_{ij} = \Delta_{ij}\Gamma_{kl} \quad (1)$$

where Ψ_{ij} represents the flux tensor, Δ_{ij} represents the homogenized coefficient of the composite and Γ_{kl} represents the field tensor.

Table 1. Fields of analyzed variables

Physical property	Elasticity	Heat conduction	Electric conduction
Material coefficient Δ_{ij}	Stiffness C_{ijkl}	Thermal conductivity K_{ij}	Electric conductivity σ_{ij}
Flux tensor Ψ_{ij}	Stress σ_{ij}	Heat flux $q,_i$	Electric current density J_i
Field tensor Γ_{kl}	Strain ε_{ij}	Thermal gradient $T_{,j}$	Electric field E_i

Qu and Cherkaoui (Chekaoui & Qu, 2006) argue that, in nature, most engineering materials are heterogeneous. These generally consist of different constituents or phases, which are distinguishable on specific scales. For engineering applications it is relevant to determine the general or effective properties of the materials analyzed on a scale of interest.

The equivalent inclusion problem, proposed by Eshelby (Eshelby, 1957.), was a milestone in the evolution of micromechanics, this idea can be extended to the generalized analysis of composites. The various methods for evaluating the effective properties of heterogeneous materials are based on the Eshelby solution for equivalent inclusion.

To determine the effective constants of the composite material, the models consider the volumetric fractions of its constituents. Quang, He and Bonnet (Quang, He, & Bonnet, 2011) established an analysis in which the equivalent inclusion method can be applied to physical problems analogous to the elastic problem, such as: electrical conduction, thermal conduction, magnetism, diffusion and porous media flow.

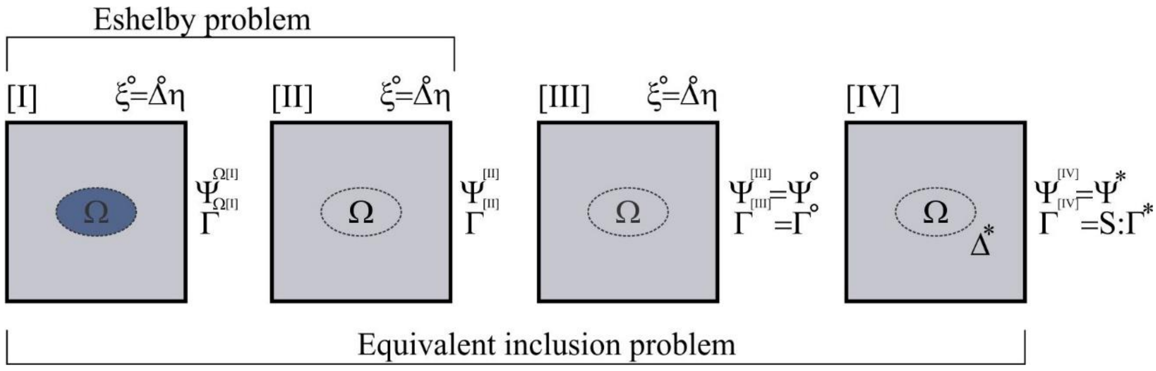
With this, the Eshelby tensors can be obtained according to the proposed variable. For example, for heat conduction and electrical conduction analysis, one can define, according to the inclusion format, the respective component values.

The basic equations of the equivalent inclusion problem (Figure 1) are described for a solid subjected to a homogeneous boundary condition in the field tensor (Γ_{Ω}). Its condition has a relation with the perturbation field (ξ^0), both outside the ellipsoid and inside it, and it can be obtained as a function (Equation 2) of an external perturbation (forces, displacements, temperature, flow etc).

$$\Gamma_\Omega = \mathbb{R}: \xi^0 \quad (2)$$

where $\mathbb{R}$ is the location tensor of the inclusion ξ^0 in the Ω domain.

Figure 1: The equivalent inclusion problem.



The flux tensor (Ψ_Ω) in the specific inclusion domain can be described as (Equation 3):

$$\Psi_\Omega = \Delta_\Omega: \mathbb{R}: \xi^0 \quad (3)$$

where Δ_Ω is material coefficient of the inclusion.

All the micromechanics models are based on the simplified idea for the location tensors. The order of the tensors $\mathbb{R}$ and $\mathbb{M}$, of the tensor $\mathbb{S}^\Omega$, as well as their construction, depend on the analysis to be performed, the geometry of the inclusion and the respective materials that make up the matrix and the inclusion. These location tensors (Equation 4), in the particular case of mechanical analysis, are known as Hill concentration tensors.

$$\mathbb{R} = [\mathbb{I} + \mathbb{S}^\Omega: \Delta^{-1}: [\Delta - \Delta^\Omega]]^{-1}$$

$$\mathbb{M} = [\mathbb{I} + \mathbb{S}^\Omega: \Delta^{-1}: [\Delta - \Delta^\Omega]]^{-1}: \Pi \quad (4)$$

$$\Pi = \Delta^{-1}$$

where $\mathbb{I}$ is the identity tensor, $\mathbb{S}^\Omega$ is the Eshelby tensor for the inclusion, Δ is the material coefficient of the matrix and Δ^Ω is the material coefficient of the inclusion.

In a simplified way, in this paper, the Eshelby tensors are used to analyze the elastic problem, presented by Nemat-Nasser (Nemat-Nasser, S., & Hori, 1993) and as presented by Withers (Withers & J., 2000), Hatta and Taya (Hatta & Taya, 1986), the Eshelby tensors for the thermal conductivity problem can be found, in a simplified way, for the spherical shape, with the following components $S_{ii}\ (\text{no sum}) = \frac{1}{3}$. For all other, $S_{ij} = 0$.

The homogenization methods found in the literature stand out for an analysis of the microstructure of composites. In this case, the concrete is analyzed, which is a material of great importance for the applications used. With this, the consideration that concrete is a composite material can be understood through the distribution of its constituent phases. In this way, it is possible to evaluate the elastic and thermal properties, homogenized according to the above.

3 Applications to Homogenization of Lighweigt Concretes

By definition, the concrete is considered lighweight when constituted by lightweight aggregates or in the combination of conventional aggregates and lightweight ones. Real *et al.* (Real, Bogas, Gomes, & Ferrer, 2016) comment that the lighweight concrete, due to its thermal properties, it presents as an alternative to the conventional concrete for improving the thermal comfort in building. Besides, one can use this material in a more effective way, due to this dead load reduction and the enviromental well-being promotion and sustainability.

Mehta and Monteiro (2014) relate the various characteristics involved in concrete's microstructure. Being a heterogeneous material, its composition and each phase properties individually influenciates in the composite properties. In a macrocospic level, the concrete can be considered as a biphasic material, consisting of aggregates particules (inclusions) dispersed in a cement paste (matrix). Nonetheless, in a microscopic level, the complexities become evidents. For example, in some ares of analyses, the hidrated cement paste appears to be more dense than the aggregates, while in others it appears to be highly porous.

The consideration of interfacial transition zone (ITZ) is essencial for the correct representation of concrete microstructure. According to Sharma and Bishnoi (Sharma & Bishnoi, 2020), this phase is generally considered the weaker than the other two. This way, the distribution of all the phases should be considered in the concrete modeling. Despite the ITZ is extremely important, some researchers use the micromechanical models for two-phase composites when the concrete is lightweight, high-strenght or when the coarse aggregate is porous enough to absorv the hidration water, as quoted by (Li, Li, & Wang, 2019.).

4 Thermal homogenization models

It is highlighted in the homogenization models analyzed in this work, the dilute suspension, generalized self-consistent and Mori-Tanaka models. All of them are described in (Chekaoui & Qu, 2006). Further analytical models not based in micromechanics, like Maxwell-Eucken and Campbell are presented in (Xu, et al., 2016).

Starting from the assumptions of biphasic composites, the recurrence equations are constructed for the evaluation of homogenization models presented in this paper. The formulation of the models should be observed in (Nemat-Nasser, S., & Hori, 1993),(Eshelby, 1957.), (Mori & Tanaka, 1973), (McLaughlin, 1977), (Christensen & Lo, 1979), (Benveniste, 1987), . In Table 2 are presented the following equations.

Table 2. Homogenization models

Models	Equation Δ^{H}
Mori-Tanaka	$\Delta_{\mathrm{m}}:\left[\mathbb{I}+f_i(\mathbb{S}-\mathbb{I}):[(\Delta_{\mathrm{m}}-\Delta_{\mathrm{i}})^{-1}:\Delta_{\mathrm{m}}-\mathbb{S}]^{-1}\right]:[\mathbb{I}+f_i\mathbb{S}:[(\Delta_{\mathrm{m}}-\Delta_{\mathrm{i}})^{-1}:\Delta_{\mathrm{m}}-\mathbb{S}]^{-1}]^{-1}$
Generalized Self-Consistent	$\frac{1}{4}[(3f_i-1)\Delta_{\mathrm{i}}+(3(1-f_i)-1)\Delta_{\mathrm{m}}+\sqrt{(3f_i-1)\Delta_{\mathrm{i}}+(3(1-f_i)-1)\Delta_{\mathrm{m}})^2+8\Delta_{\mathrm{m}}:\Delta_{\mathrm{i}}}]$
Dilute Suspension	$\Delta_{\mathrm{m}}+f_i(\Delta_{\mathrm{i}}-\Delta_{\mathrm{m}}):[\mathbb{I}+(\mathbb{S}:\Delta_{\mathrm{m}}{}^{-1}):(\Delta_{\mathrm{i}}-\Delta_{\mathrm{m}})]^{-1}$
Series	$\Delta_{\mathrm{i}}f_i+\Delta_{\mathrm{m}}(1-f_i)$
Parallel	$\left[\Delta_{\mathrm{i}}{}^{-1}f_i+\Delta_{\mathrm{m}}{}^{-1}(1-f_i)\right]^{-1}$
Hashin lower limit	$[\Delta_{\mathrm{m}}:\Delta_{\mathrm{i}}+2\Delta_{\mathrm{m}}:(\Delta_{\mathrm{m}}(1-f_i)+\Delta_{\mathrm{i}}f_i)]:[2\Delta_{\mathrm{m}}+\Delta_{\mathrm{m}}f_i+\Delta_{\mathrm{i}}(1-f_i)]^{-1}$
Hashin upper limit	$[\Delta_{\mathrm{m}}:\Delta_{\mathrm{i}}+2\Delta_{\mathrm{i}}:(\Delta_{\mathrm{m}}(1-f_i)+\Delta_{\mathrm{i}}f_i)]:[2\Delta_{\mathrm{i}}+\Delta_{\mathrm{i}}(1-f_i)+\Delta_{\mathrm{m}}f_i)]^{-1}$

where $\Delta^{\mathbf{H}}$ is the homogenized composite coefficient, $\Delta_{\mathbf{m}}$ is the matrix coefficient, $\mathbb{I}$ is the identity tensor, f_i is the volumetric fraction of the inclusion, $\mathbb{S}$ is the Eshelby tensor and $\Delta_{\mathbf{i}}$ is the inclusion coefficient.

The mean-fields models for elastic homogenization analysis can be used for the extension of the problem for thermal analysis of composites. The determination of the coeficientes of thermal conductivity and thermal expansion, in effective terms, can be used based in Hill's concentration tensors.

It is emphasized that all the methods ignore the spatial distribution of heterogeneities, it means that is assumed that it has a uniform distribution of inclusions. However, the shapes and orientations of heterogeneities are considered by the means of Eshelby tensor.

This way, it stands out the effective properties predicted by the homogenization models do not depends on the inclusions size. The interactions between the inhomogeneities are taken in consideration in differents ways for the differents approaches.

In general, the dilute suspension model is consistent for small volumetric fractions of inclusions, while the others are applicable for the differents ranges of inclusion volumes. Lee *et al* (2018) consider that the homogenization theories are acceptable for composites that the volumetric fractions of the inclusions are less than 20%.

Lee comment the complexity of obtaining the thermal conductivity matrix, that it is anisotropic, it means that the thermal conductivity varies with the direction of the heat flux applied to the matrix. It also can be noted that the interfacial thermal resistance can reduce the thermal conductivity of the composite (Lee, Lee, Ryu, & Ryu, 2018).

5 Thermoelastic homogenization models: Levin's formula

For the thermal expansion coefficients homogenization analyses, (Zhou, Shu, & Huang, 2014) mention that the raw materials, aggregate type, moisture, age and other factors influence in the composite effective coefficient. In the specific case of lightweight concrete, it is assumed the hypotesis of porous material, so it can be checked that implies in a reduction of the effective coefficient.

Levin (1967) proposed a correlation for determining the effective thermal expansion coefficient, considering the contribution of the stress concentration tensor of Hill (Lages & Marques, 2020) (Eq. 5):

$$\bar{\alpha} = \sum_{\lambda=1}^{N} f_{\lambda} \cdot \alpha^{(\lambda)} \cdot B^{(\lambda)} \qquad (5)$$

where $\bar{\alpha}$ is the vector of effective thermal expansion coefficient for a composite constituted for N phases, $\alpha^{(\lambda)}$ is the vector of thermal expansion coefficient for each phase and $B^{(\lambda)}$ is the stress concentration tensor for each phase (Levin, 1967).

Uygunoglu e Topçu (Uygunoglu & Topçu, 209) relate that the values of thermal expansion coefficients of lightweight aggregates are accepted between $7 \cdot 10^{-6}$ and $13 \cdot 10^{-6}$ °C^{-1}. The typical values of plain concrete produced with normal weight aggregates are, generally, between $7.4 \cdot 10^{-6}$ and $13.1 \cdot 10^{-6}$ °C^{-1}. It shows that lightweight concrete tends to a lower effective coefficient than the normalweight ones.

In the prediction model, using the Levin's formula (Lages & Marques, 2020), one should note that the inclusions, considered as materials of zero stiffness (Young modulus closes to zero), do not influences in the concrete's thermal expansion coefficient. The dependence on the mechanical problem on the recurrence equation, implies in a minimum variation in the effective coefficient. It means that the lightweight concrete has approximate the same thermal expansion coefficient as the normal weight concrete.

6 Results and Discussions

The lightweight concrete analyzed in this work has a range of density between 1120 to 1920 kg/m³, according to ACI 213 (ACI-213R-03, 2003). Thus, the aggregate type, its shape and dimensions, influences in the composite behavior. The particularities of lightweight concrete assumptions allow the utilization of micromechanics theory for modeling as a porous material.

In this paper, it is evaluated the effectives thermal conductivity and thermal expansion coefficients of lightweight concrete, comparing the following possible situations: EPS particles inclusion, expanded clay particles inclusion and air-entraining admixture simulating as the pores inclusion.

6.1 Microstructural aspects of lightweight concrete

For the analyses of effective thermal conductivity of concrete, (She, Zhao, Cai, Jiang, & Cao, 2018), (Sayadi, Tapia, Neitzert, & Clifton, 2016), (Xu, et al., 2016), (Wei, Yiqiang, Yunsheng, & Jones, 2013) presented the caracterization of the concrete with lightweight aggregates, particularly, the concrete with particples of expanded polysthirene (EPS).

Asadi *et al.* mention that the porosity has a significant role in thermal conductivity of composites. It is realized the authors made an extensive data for correlations of thermal properties of concrete. Typical values can also be seen in (Honório, Bary, & Benboudjema, 2018), (Asadi, Shafigh, Hassan, & Mahyuddin, 2018).

In the concrete properties, it is checked that there is a dependence on the cement contente, the density, the mineralogical characteristic of the aggregate, the admixtures and the temperature. So, it all can be related to the parameters evaluation in the analysis of the microstructure of concrete.

6.2 Phases properties

Every homogenization step receives as an input the matrix and the randomic inclusion, and it provides as output the material with the homogenized properties. The materials' properties used for this composite construction are defined in Table 3.

Table 3. Phases properties of composite

Phase	Density (kg/m³)	Thermal conductivity coefficent (W/(m·K))
Concrete	1900	0.900

EPS	30	0.041
Pores	-	0.025
Expanded clay	400	0.160

Asadi *et al.* (2018) proposed a fit equation (Equation 6) for thermal conductivity of ligthweight concrete, since this is a function of the material density (ρ). This comparative study was proposed based in 185 experimental results available in literature. It can be checked that this equation and the one recommended in the ACI 213 (ACI-213R-03, 2003) are both adherent to densities below 1500 kg/m³.

$$k_{exp} = 0.0625 \cdot e^{0.0015 \cdot \rho} \quad (6)$$

This way, it can be defined the density of analyzed concrete, and using this information, it can be associated the volumetric fraction of inclusions considered in this concrete manufacture. This concept, as can be seeing in Miled (Miled, Sab, & Le Roy, 2007), it is associated with the macroporosity (Equation 7):

$$f_i = \frac{\rho - \rho_c}{\rho_i - \rho_c} \quad (7)$$

where ρ_i is the density of the inclusion and ρ_c is the density of the concrete and ρ is the density of the lighweight concrete.

6.3 Effective thermal conductivities

The thermal conductivity values of lightweight concrete with different inclusions: expanded polystyrene (Figure 2), pores (Figure 3), expanded clay (Figure 4) do not change drastically, however in percentage terms the numerical error compared to the experimental data increases drastically when the inclusions are increased, reaching error peaks of 30% for any type of inclusion.

The models that establish the Hashin, series and parallel limits are important for verification because they delimit the region that the values are acceptable, for this reason, they can't be used to check any fit to experimental data.

It was expected that the dilute suspension model would not adhere to the Equation 6., since it has limitations of low volume fractions in its formulation, so that when increasing the volume fraction, the values will move away from the expected.

From the analysis, it could be checked that the Mori-Tanaka model obtained identical values to the Hashin upper limit, not adhering well to the experimental data. The Generalized Self-Consistent (GSC) was the one that obtained the best results.

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Figures 2, 3 and 4 illustrate the relationship between the density of the inclusion material and its respective thermal conductivity. The volume fraction of inclusion at the time is obtained by Eq. 7.

Figure 2: The relationship between density and thermal conductivity – EPS

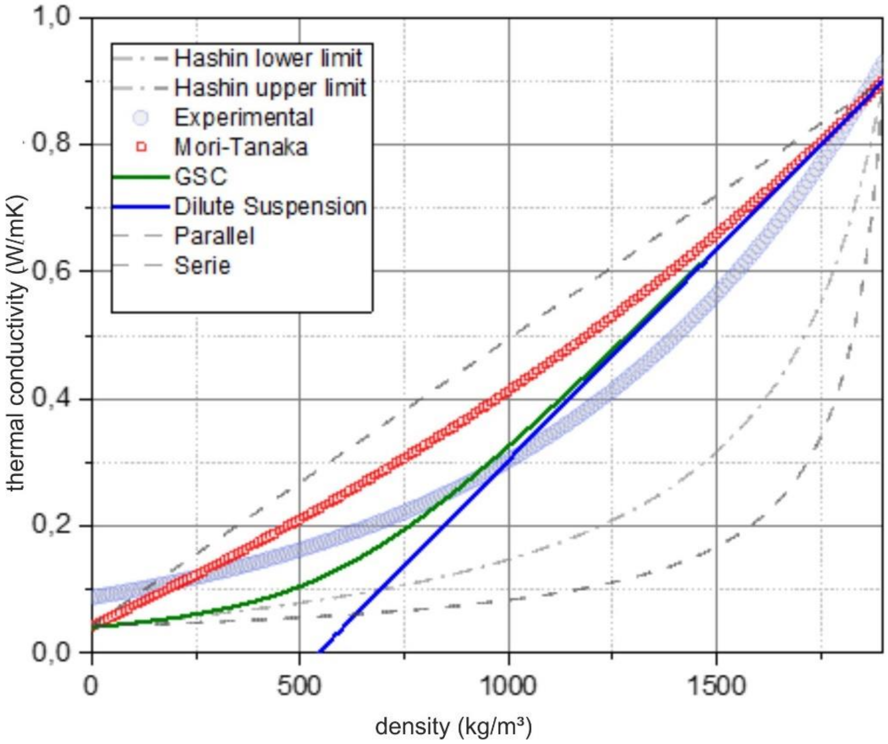


Figure 3: The relationship between density and thermal conductivity – PORES

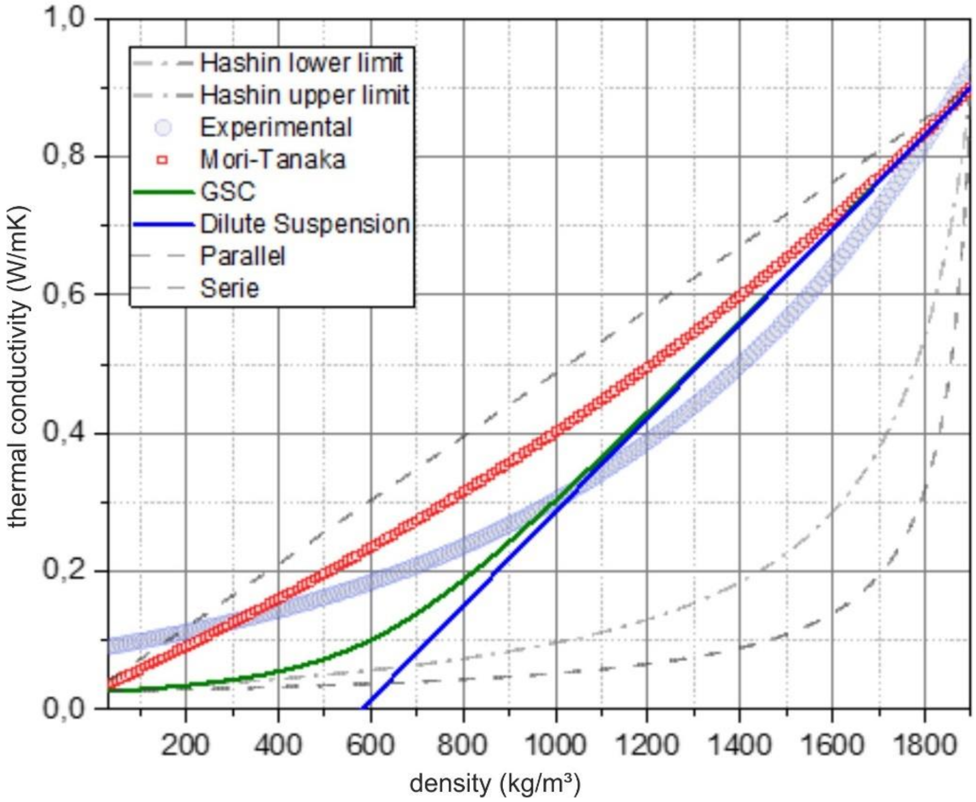
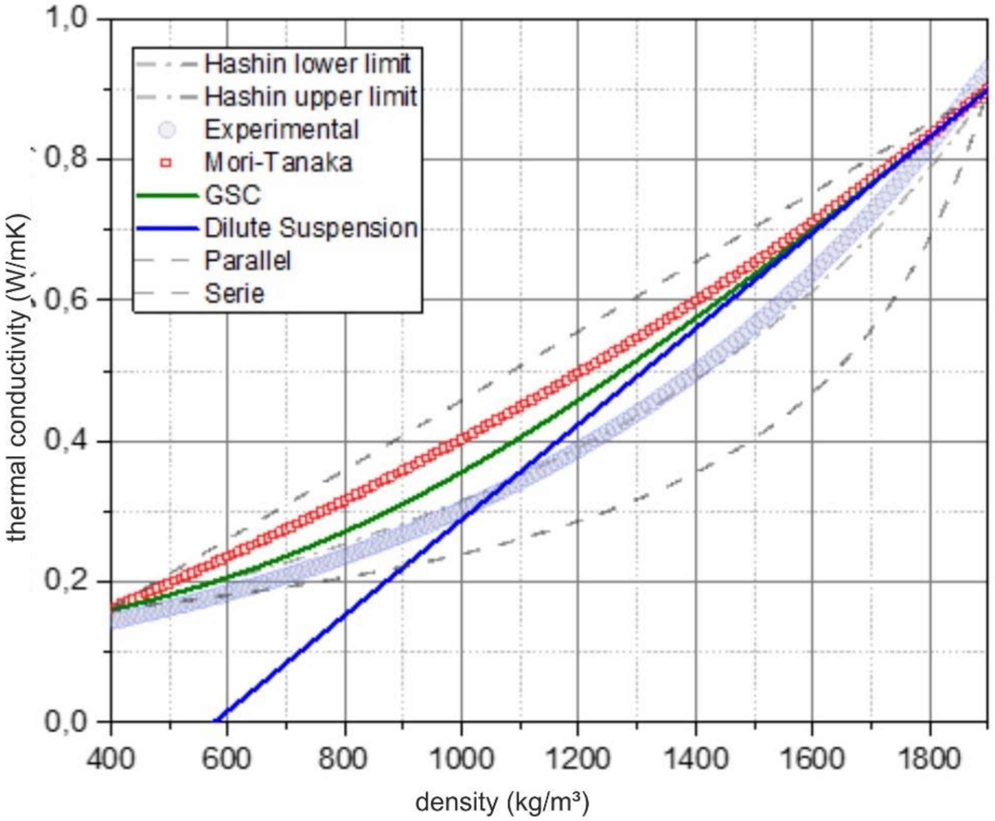


Figure 4: The relationship between density and thermal conductivity – EXPANDED CLAY



When concrete has an overall density ranging between 900 kg/m³ 1900 kg/m³ the best homogenization results are observed, ranging from zero to 15% of the value estimated by the experimental data. When the inclusions are increased to the point that the overall density of the composite drops from 900 kg/m³, numerical results increase, leading to unacceptable modeling errors.

7 CONCLUSIONS

The proposed framework for predicting the thermal properties of lighweight concrete is related to the mean-fields theories of micromechanics. It is empashized that the experimental data of the phases properties is the most important step for the homogenization analysis. Its characterization and behavior, which depends on the specific test conditions and the desired characteristics of the concrete, is associated with a large variability within homogenization numerical models parameters, that bring some uncertainties in the adopted models.

The numerical errors of the homogenization models for thermal conductivity, that in the analyses only varies with the density of the concrete, is a possibility to measure an estimative of the correct approximate behavior of the composite. The better approximation in all the models should be noted when the density of the composite is close to the concrete considered as matrix (1900 kg/m³). Outside this range, for example, in densities between 900 kg/m³ and 1100 kg/m³, GSC model agree with the correspondent homogenized coefficient predicted by the fit equation proposed by Asadi.

The thermal properties of the lightweight concrete analyzed in this paper plays an important role in the performance of the system. Reducing the dead load in a structure is always a target to minimize cost and increase safety. It is can be checked that this strategy can be used to help engineers designing materials to simulate the suitability of thermal performance to get a better comfort in a buildings. In the specific case of concrete, the dosage of inclusions (or inhomogeneities), using the framework presented in this paper, is a possibility to obtain lighweight concrete respecting a required level of thermal performance.

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