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ORIGINAL ARTICLE

Concrete modeling using micromechanical multiphase models and multiscale analysis

Modelagem do concreto usando modelos micromecânicos de múltiplas fases e análise multiescala

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Abstract: Concrete in its macrostructure is a multiphase cementitious composite material, however, by reducing its scale, it is possible to identify the phases that compose it, among the phases are those embedded in the microscale: the hydrated silicates, in the mesoscale: the cement paste, transition zones and aggregates and in the macro phase: the composite itself. Modeling this type of material with two-phase micromechanical models is common in the literature, but there are already proven limitations that two-phase models can provide high modeling errors and are not recommended for this type of study. Faced with this problem, an alternative would be to use multiple-phase models, combined with a multiscale perspective in an attempt to minimize the error in modeling this material. The present paper models the concrete in two different constructions: without an interfacial transition zone and with the inclusion of the interfacial transition zone, verifying the modeling error when neglecting this important phase. The entire homogenization process is performed using the decoupled multiscale technique, obtaining results that rule out the use of two-phase models and methodologies that do not evaluate the interfacial transition zone in conventional concrete. The results obtained with the use of multiple-phase models reduced the relative error to practically zero (compared to experimental tests), demonstrating that micromechanics can be a concrete modeling tool provided that the multiscale process considers as many as possible phases and robust models that take this nature into account.

Keywords: multiscale modeling, micromechanics, concrete.

Resumo: O concreto em sua macroestrutura é um material compósito cimentício multifásico, contudo ao se reduzir sua escala consegue-se identificar as fases quem compõe o mesmo, dentre as fases estão as embutidas na microescala: os silicatos hidratados, na mesoescala: a pasta de cimento, zonas de transições e agregados e na fase macro: o próprio compósito. Modelagens desse tipo de material com modelos micromecânicos bifásicos são comuns na literatura, porém existe limitações já comprovadas de que modelos de duas fases podem aferir erros altos a modelagem não sendo recomendado para esse tipo de estudo. Diante dessa problemática, uma alternativa seria empregar modelos de múltiplas fases, aliado a uma perspectiva multiescala na tentativa de minimizar o erro na modelagem desse material. O presente trabalho modela o concreto em duas construções distinta: sem zona de transição interfacial e com a inclusão da zona de transição interfacial, verificando o erro de modelagem à negligência essa importante fase. Todo processo de homogeneização é realizado utilizando a técnica multiescala desacoplada obtendo resultados que descartam a utilização de modelos bifásicos e metodologias que não avaliam a zona de transição interfacial em concretos convencionais. Os resultados obtidos com a utilização de modelos de múltiplas fases reduziram o erro relativo a praticamente zero (em comparação com ensaios experimentais), demonstrando que a micromecânica pode ser uma ferramenta de modelagem do concreto desde que o processo multiescala leve em consideração o maior número possíveis de fases e modelos robustos que levem em conta essa natureza.

Palavras-chave: modelagem multiescala, micromecânica, concreto.

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1 INTRODUCTION

Multiscale modeling is a technique that has been developed over the last decades with several applications in the most varied fields of science. The idea is to simulate continuous behavior from information obtained at lower scales [1].

In his paper Fish et al. [1] he presents a review of the most interesting applications of multiscale modeling including the prediction of electrical, magnetic, and chemical properties of complex materials (for example composites).

For each application, it is possible to define the multiscale approach that will be used, explaining its advantages and disadvantages in addition to the degree of complexity inherent to its technique [2]. Multiscale modeling consists of evaluating each level and how they influence each other as the composite is built. Lloberas-Valls et al. [2] defines two types of multiscale modeling, namely: hierarchical multiscale technique and concurrent multiscale technique.

The hierarchical multiscale technique can be divided into decoupled or weak coupled, in the decoupled technique the boundary condition problem is already solved, and the effective properties are carried from one scale to another (common in micromechanical homogenization). When the problem is analyzed by weak coupling, properties can be taken from global to local scale and vice versa, and the boundary problem is not initially solved. In the concurrent multiscale technique, the different scales are solved simultaneously, maintaining the condition of equilibrium and displacements, explaining a strong coupling [2].

Given this premise of expansion of knowledge and since concrete can be considered a complex material (composite) due to its multiphase and cementitious nature, this work proposes to estimate the mechanical properties of concrete using multiscale, micromechanical modeling of mean fields, bringing as a contribution to the application of models involving multiple phases, including the interfacial transition zone, in addition to verification and comparison with classical biphasic models. To validate the multiscale modeling, a comparison is made with experimental tests.

On a macroscopic scale, concrete may be considered as a homogenous material, however, as the scale decreases (meso and microscale), it cannot be considered homogenous – it is heterogenous, explaining its respective phases relate in [3], [4], [5]. Knowing the phases that compose the concrete, its respective fractions, and how they interact with one another is fundamental to maximizing its use.

Rodrigues [6] explains that the region that comprehends the mesoscale is a target of interest for several researchers: Häfner et al. [7], Eckardt and Könke [8], Eckardt [9], Nguyen et al. [10] since this phase defines the concrete as a composite and multiphase material.

In their study, Pichler and Hellmich [11] characterize well the multiscale modeling of some phases of the concrete (decoupled technique), namely: cement paste and the process of hydration of the paste that contemplates portions of the hydrated silicates, water/capillary pores, and clinker.

Further on, multiscale modeling of concrete was proposed, contemplating an experimental campaign to validate the models previously proposed by Göbel et al. [12].

Siventhirarajah et al. [13] can go further, through a multiscale analysis reducing the cement paste in some levels, reaching the nanometric scale, evaluating the hydrated calcium silicates HCS that compose the clinker (C_3S, C_2S, C_3A, C_4AF), tricalcium silicate, dicalcium silicate, tricalcium aluminate, tetracalciumalumino ferrite, respectively. In 2004 Scrivener [14] published an important paper on the characterization and measurement of concrete phases, especially the phases that make up a cement past.

Figure 1 illustrates the multiscale diagram of concrete showing its phases and dimensions from the microscale, through the mesoscale to the macroscale [3], [4], [9], [10], [11].

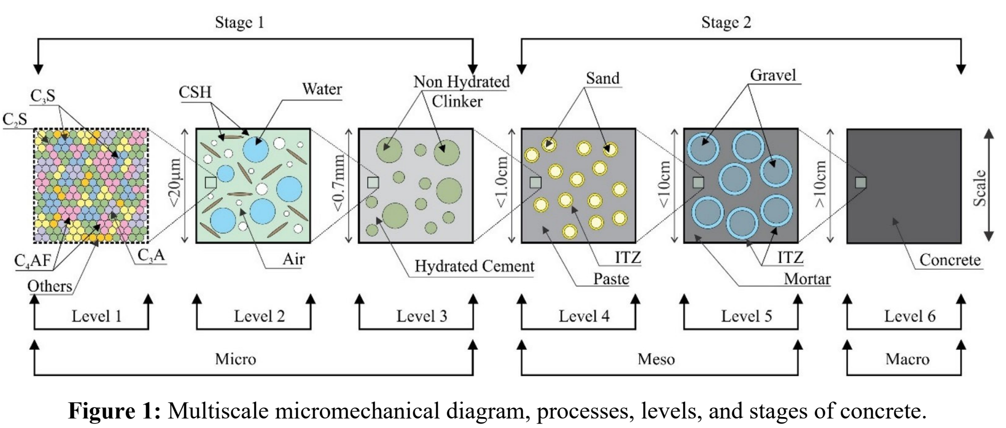


Figure 1: Multiscale micromechanical diagram, processes, levels, and stages of concrete.
Source: Author, adapted from Bernard et al. [3], Siventhirarajah et al. [13].

Siventhirarajah et al. [13] subdivides the analysis of concrete into two stages – the first stage being responsible for integrating models of humidity, thermodynamics, and the hydration of the cement paste to evaluate the volumetric fractions of the comprehended phases between levels 1 to 3 (microscale). With the respective fractions and properties of the phases of stage 1, it is possible to estimate the property of the cement paste. The second stage is related to the mechanical evaluation of the composite (meso and macroscale), comprehending the phases of the sand and gravel, the respective interfacial transition zone (ITZ), and mortar.

In this stage (< level 6), the concrete can be understood as a composite, cementitious and multiphase material, which makes it complex, and simplified tests cannot evaluate its behavior.

Still, at level 5, the literature has long tried to understand the participation of each component of this mixture in the final characteristics of the composite, much has already been discovered, since the great influence of inclusions [15], [16], [17], [18], as well as a third, more fragile phase located at the matrix-inclusion interface (interfacial transition zone), which is difficult to measure but which has already been extensively tested by several techniques [19], [20], [21].

Silva [18] highlight the relationship between these phases and the possible behavior of each one when subject to request. When the inclusion phase is dominant in the stiffness of the composite, the matrix phases and the transition zone deform to a greater extent, which is probably the preferred path for cracking and fracturing of the composite.

However, even if the interfacial transition zone generated by the gravel is included, there are other phases, highlighting: sand pores, interfacial transition zone generated by sand, and even smaller phases such as non-hydrated clinker, hydrated silicates, among others, passing through all the levels shown in Figure 1.

Each of these phases has distinct properties and volumetric fractions and good modeling is directly associated with the characterization of each one of them. This dependence on concrete modeling as a function of the number of phases is remedied with a multiscale modeling using multi-phase micromechanical models, as proposed in this article.

2 INITIAL CONSIDERATIONS ON COMPOSITE HOMOGENIZATION

2.1. Representative Volume Element

A given body admitted homogenous and continuous in its macro-structure when reduced to a sufficiently small scale, does not behave as homogenous material, but as heterogeneous one, besides presenting discontinuities.

The literature brings several definitions about which volume will be representative of its macro-scale as seen in [11], [22], [23], [24], [25], [26].

Stroven et al. [25] discourses about the diverse definitions related to RVE (representative volume element), proposing a form of its measuring, taking into consideration a statistic dispersion associated with a specific property, when its scale is reduced. Still, in the paper [25] the following definitions are highlighted:

Hashin [22] admits that a volume is representative if it contains all of the phases that characterize the microstructure of the heterogeneous material studied and a sufficient number of these phases for the corresponding mean properties to the RVE to be independent of the applied conditions of contour, once these conditions are macroscopically uniform, or, in other words, the values oscillate around a mean value with a small standard deviation, becoming insignificant at a small distance of the surface.

Drugan and Willis [23] indicate that the representative volume element is associated with the smaller volume that can represent the mean properties of the composite.

Ostoja-Starzewski [24] defines RVE in two situations: when the system is periodic in its micro-structure and there is a cell that represents it, and in the second case when there is a volume (great enough) that can incorporate several phases in its micro-structure, presenting homogenous structures.

The reference quoted above about RVE differs a little, however, RVE is always considered inferior to the macroscale of the composite, which can represent its phases and must have little dispersion in the evaluation of its properties when its volume is disturbed [25].

Drago and Pindera [26] bring a definition of RVE as being a heterogenous system in its micro-structure, where when the specific contour conditions are applied for each representative volume, the answer does not differ from the material in its macroscale. Drago and Pindera [26] still explained the concept of the unitary cell of repetition, which is widely used when the problem has a condition of periodical contour.

In their review about RVE the authors described several studies that aimed at the characterization of the representative volume element, especially for concretes, once they were trying to know if the samples evaluated in fact could represent the composite. These studies established a parametric analysis of the volume and its phases submitted to several conditions of homogenous contour. These investigations tried to define the number of inclusions contained in the RVE that would be sufficient for the evaluation of the properties of the composite.

Pichler and Hellmich [11] define representative volume element due to the analysis scales. In a simplified manner, the definitions quoted above continue to be valid, however, there may be a representative element inside another representative element to be able to evaluate its properties on an even smaller scale.

Suppose that a representative volume element on scale A, composed of $n1$, $n2$, …, nm

phases, in such a way that when the analysis scale is reduced to B, it is possible that some of its $n1$, $n2$, …, nm, phase have to be represented by other $k1$, $k2$, …, km, phases, expanding the range of phases for the multi-scale analysis, well defined in concrete. e.g.: Pichler and Hellmich [11] and approached in this study.

Micromechanical analyzes are normally conducted based on the concept of a representative volume element (RVE). The composite material can be understood as the sum of the matrix volume with the sum of the volume of all the inclusions, which can be voids, materials, cracks, etc [27]. Equation 1, below, represents this method.

$$V = V_m + \sum_{\alpha=1}^{n} V_i \quad (1)$$

Where V_m is the volume of the matrix, V_i is the volume of inclusions, and V is the total volume of the representative element. When taking the ratio between the matrix volume and the total volume, as well as the volume of inclusions and the total volume, the following volumetric fractions are obtained, considering Equations 2 and 3, respectively.

$$f_m = \frac{V_m}{V} \quad (2)$$

$$f_i = \frac{1}{V}\sum_{i=1}^{n} V_i \quad (3)$$

Volumetric fractions are extremely important in this type of analysis. The simplest proposes a weighted average as a function of fractions, of properties for global analysis, also known as the rule of mixtures. Over time, several methods were developed to solve the micromechanical problem, highlighting the Equivalent Inclusion Method, developed by Eshelby [28], one of the great contributions to the development of the micromechanics of effective media.

From the method proposed by Eshelby [28] other methods were developed, highlighting: Self Consistent [29], Mori-Tanaka [30], and Differential Scheme [31], among others.

The study of the micromechanics of effective media admits the hypothesis that the representative stresses and strains of a composite material (matrix + inclusions) can be represented by the average of stresses and strains in the representative volumes of each phase. Based on this principle, the total average stress, in the matrix and the inclusions, can be expressed by (Equations 4-6):

$$\overline{\sigma} = \frac{1}{V}\int_V \sigma(x)dv \quad (4)$$

$$\overline{\sigma}_m = \frac{1}{V_m}\int_{V_m} \sigma(x)dv \quad (5)$$

$$\overline{\sigma}_i = \frac{1}{V_i}\int_{V_i} \sigma(x)dv \quad (6)$$

Knowing that:

$$\int_V \sigma(x)dv = \int_{V_m} \sigma(x)dv + \sum_{i=1}^{n}\int_{V_i} \sigma(x)dv \quad (7)$$

replacing Equation 7, in Equation 4 there have been (Equation 8):

$$\overline{\sigma} = f_m\overline{\sigma}_m + \sum_{i=1}^{n} f_i\overline{\sigma}_i \quad (8)$$

Arrived at an expression that can determine the total average stress as a function of the stresses in the matrix and the inclusions and their respective volumetric fractions. Assuming that V is a representative volume, it can be stated that the average total stress $\overline{\sigma}$ is equal to the effective stress in the material $\langle\sigma\rangle$. Similarly, we have the total mean strain, in the matrix and the inclusions are given by the Equations 9-11:

$$\overline{\varepsilon} = \frac{1}{V}\int_V \varepsilon(x)dv \quad (9)$$

$$\overline{\varepsilon}_m = \frac{1}{V_m}\int_{V_m} \varepsilon(x)dv \quad (10)$$

$$\overline{\varepsilon}_i = \frac{1}{V_i}\int_{V_i} \varepsilon(x)dv \quad (11)$$

Knowing that:

$$\int_V \varepsilon(x)dv = \int_{V_m} \varepsilon(x)dv + \sum_{i=1}^{n}\int_{V_i} \varepsilon(x)dv \quad (12)$$

replacing Equation 12, in Equation 9 there have been (Equation 13):

$$\overline{\varepsilon} = f_m\overline{\varepsilon}_m + \sum_{i=1}^{n} f_i\varepsilon_i \quad (13)$$

Assuming that matrix and inclusions are elastic materials. So, it can be said that (Equations 14-16):

$$\langle\sigma\rangle = \overline{\mathbb{C}}:\langle\varepsilon\rangle \quad (14)$$

$$\langle\sigma_m\rangle = \mathbb{C}_m:\langle\varepsilon_m\rangle \quad (15)$$

$$\langle\sigma_i\rangle = \mathbb{C}_i:\langle\varepsilon_i\rangle \quad (16)$$

Where, $\overline{\mathbb{C}}$, $\mathbb{C}_m$, and $\mathbb{C}_i$ are respectively the global constitutive tensor, the matrix constitutive tensor, and the inclusion constitutive tensor, being the same fourth-order tensors. If the material is linear elastic, the global constitutive tensor is constant.

The concentration tensors of a composite are tensors that relate the average stresses and strains in the composite with the matrix and the inclusions. Substituting Equations 14-16 to Equation 8, we obtain (Equations 17-18):

$$f_m\mathbb{C}_m:\langle\varepsilon_m\rangle = \overline{\mathbb{C}}:\langle\varepsilon\rangle - \sum_{i=1}^{n} f_i\mathbb{C}_i:\langle\varepsilon_i\rangle \quad (17)$$

$$f_m\mathbb{C}_m:\frac{1}{V_m}\left[\int_V \varepsilon(x)dv - \sum_{i=1}^{n}\int_{V_i} \varepsilon(x)dv\right] = \overline{\mathbb{C}}:\langle\varepsilon\rangle - \sum_{i=1}^{n} f_i\mathbb{C}_i:\langle\varepsilon_i\rangle \quad (18)$$

With a little algebra one can arrive at (Equation 19):

$$(\overline{\mathbb{C}} - \mathbb{C}_m):\langle\varepsilon\rangle = \sum_{i=1}^{n} f_i(\mathbb{C}_i - \mathbb{C}_m):\langle\varepsilon_i\rangle \quad (19)$$

This equation relates the constitutive tensors of the matrix, the inclusion and the global tensor, the global deformations, and the inclusion.

2.2. The Eshelby Problem

In 1957 Eshelby [28] proposed to determine the elastic field of an ellipsoidal inclusion in a solid (Figure 2).

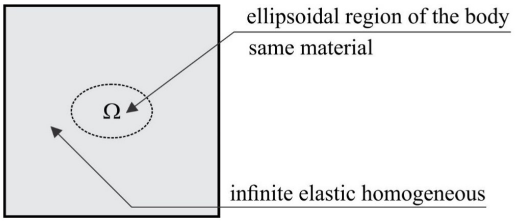


Figure 2: Esheby's inclusion problem

It is assumed that the Ω region undergoes a geometric transformation so that in the absence of the material that surrounds the ellipse region it would correspond to a homogeneous deformation. In this hypothesis, Eshelby was able to assess what the elastic fields would be like inside and outside the ellipsoidal region. To exemplify Eshelby's strategy, initially, the ellipsoidal region, where the strain is initially zero, is removed, and a homogeneous strain is applied as shown in Figure 3.

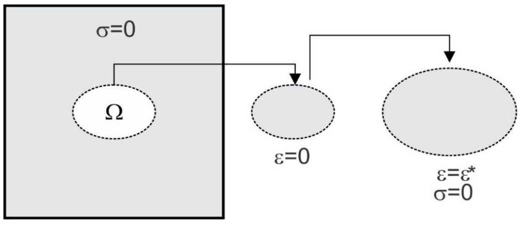


Figure 3: Eshelby's problem strategy.

The next step is to apply external forces to the region so that it returns to its initial volume. When these external forces are applied, the volume of the ellipsoidal region decreases, however, a tension field is associated with this force in the body (Figure 4).

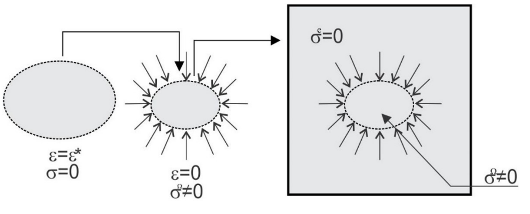


Figure 4: Eshelby's problem strategy.

The next step consists of returning to the ellipsoidal region, now with a tension field in the region of the representative element, removing the external actions that surrounded the ellipsoidal region, as can be seen in Figure 5.

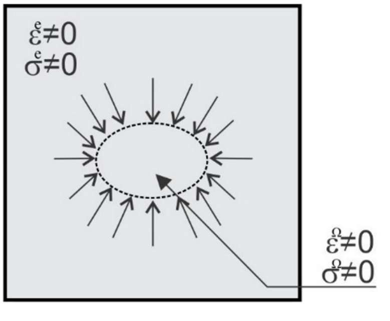


Figure 5: Eshelby's problem strategy.

Eshelby [28] states that within the ellipsoidal inclusion Ω, the stresses and strains are constant but dependent on the geometry of the inclusion. With this, we define the [28] relation between the deformations in the ellipsoid and the deformation imposed on the system by a transformation tensor, called the Eshelby tensor ($\mathbb{S}$), in the form:

$$\varepsilon^{\Omega} = \mathbb{S}^{\Omega}\varepsilon^{*} \tag{20}$$

The assembly of the Eshelby tensor can be seen in the original paper [28]. With the same strategy mentioned above, it is enough to modify the property of the ellipsoid to arrive at the equivalent inclusion method that was the precursor of the mean-fields micromechanics.

2.3. Composite Homogenization Models

There are homogenization models that have the purpose of establishing limits, the best known being the rule of mixtures (Reuss and Voigt Model) [32] and the Hashin-Shtrikman models [33]. Models should not be used to estimate the homogenized properties of composites, as they have several simplifying hypotheses such as the constant stress or strain field, or the combination of the two states, another simplification occurs in the non-evaluation of the interaction between the particles, among others.

To circumvent the limitations of limit models, methods based on the Eshelby equivalent inclusion problem stand out, the best known being the Mori-Tanaka model [34], before the paper of Mori and Tanaka [34], Hill [35] proposed the “Self-Consistent” model, which was later expanded by Christensen and Lo [27]. Also, noteworthy are the paper of Benveniste [29], with the model of equivalent inclusion [30], and his model called “Differential Scheme” and the model “Double Inclusion” [21].

Kaw [32] divides composite homogenization models into the mechanic of materials, semi-empirical models, and elasticity theory models. The present paper adopts as a reference this subdivision proposed by Kaw [32] adding the models that are derived from the mean-fields micromechanical formulation.

Table 1: Characteristics of homogenization models.

Models	Particulars and recurrence equation	Source
Reuss	Its limitation is the imposition of a constant state of tension, in addition to not evaluating the interaction between inclusions	[36]
	$\mathbb{C}^{\mathrm{H}} = \mathbb{C}_m : \mathbb{C}_i : [\mathbb{C}_i(1-f_i) + \mathbb{C}_m f_i]^{-1}$	
Voigt	Its limitation is a constant of strain state, in addition to not evaluating the integration between the inclusions	[32]
	$\mathbb{C}^{\mathrm{H}} = \mathbb{C}_m(1-f_i) + \mathbb{C}_i f_i$	
Hashin	It does not estimate constant stress and strain fields, instead, it estimates auxiliary fields representing a variation of the reference solution. When the formulation of the energy obtained is maximized, the upper limit is found and when it is minimized, the lower limit is found.	[33]
	$K^{-} = K_m + \left[\dfrac{f_i}{\left[\dfrac{1}{K_i - K_m} + \dfrac{3(1-f_i)}{3K_m + 4G_m}\right]}\right]$	
	$K^{+} = K_i + \left[\dfrac{1-f_i}{\left[\dfrac{1}{K_m - K_i} + \dfrac{3f_i}{3K_i + 4G_i}\right]}\right]$	
	$G^{-} = G_m + \left[\dfrac{f_i}{\left[\dfrac{1}{G_i - G_m} + \dfrac{6(1-f_i)(K_m + 2G_m)}{5G_m(3K_m + 4G_m)}\right]}\right]$	
	$G^{+} = G_i + \left[\dfrac{1-f_i}{\left[\dfrac{1}{G_m - G_i} + \dfrac{6f_i(i + 2G_i)}{5G_i(3K_i + 4G_i)}\right]}\right]$	
Mori-Tanaka	It is the most used model for homogenization of composites, it considers the interaction between the particles and can be used with larger volumetric fractions.	[34]
	$\mathbb{C}^{\mathrm{H}} = \mathbb{C}_m : \begin{matrix}\{\mathbb{I} + f_i(\mathbb{S} - \mathbb{I}) : [(\mathbb{C}_m - \mathbb{C}_i)^{-1} : \mathbb{C}_m - \mathbb{S}]^{-1}\} :^{-1} \\ \{\mathbb{I} + f_i\mathbb{S} : [(\mathbb{C}_m - \mathbb{C}_i)^{-1} : \mathbb{C}_m - \mathbb{S}]^{-1}\}\end{matrix}$	
Dilute Suspension	It is limited by the amount of volumetric fraction of inclusion in the homogenization process, and can only be applied to low inclusion rates	[37]
	$\mathbb{C}^{\mathrm{H}} = \mathbb{C}_m + f_i(\mathbb{C}_i - \mathbb{C}_m) : \mathbb{A}_i$	

Table 1: Continued...

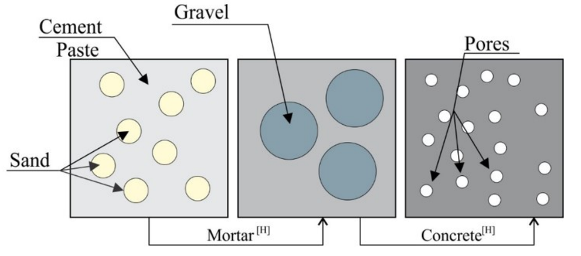
Models	Particulars and recurrence equation	Source
Self-Consistent	$\mathbb{A}_i = [\mathbb{I} - \mathbb{S}:\mathbb{C}_m:(\mathbb{C}_m - \mathbb{C}_i)]$	[35]
	$\mathbb{C}^{H}{}_{n+1} = \mathbb{C}_m + f_i(\mathbb{C}_i - \mathbb{C}_m):[\mathbb{I} - \mathbb{S}^{H}{}_n:\mathbb{C}^{H^{-1}}{}_n:(\mathbb{C}^{H}{}_n - \mathbb{C}_i)]^{-1}$	
	Step 1:	
	$\mathbb{S}^{H} = \mathbb{S}, \mathbb{C}^{H} = \mathbb{C}_m$	
	$\frac{\|\mathbb{C}^{H}{}_n - \mathbb{C}^{H}{}_{n-1}\|}{\|\mathbb{C}^{H}{}_{n-1}\|} < \delta$	
Generalized Self-Consistent	Based on the theory of elasticity, it manages to evaluate the interaction between inclusions being developed as a three-phase model, essentially it only evaluates two phases. It considers the inclusion-matrix interaction and between inclusions	[27]
	$A\left[\frac{G^H}{G_m}\right]^2 + B\left[\frac{G^H}{G_m}\right] + C$	
	A, B, and C, are constants that can be obtained in Christensen and Lo [27]	
	$K^H = \left[K_m + \frac{f_i(K_i - K_m)(3K_m + 4G_m)}{3K_m + 4G_m + 3(1 - f_i)(K_i - K_m)}\right]$	
Differential Scheme	Unlike other methods that assume an inclusion immersed in an infinite matrix, the differential scheme works with incremental doses of inclusions.	[30]
	$\mathbb{C}^{H}{}_{n+1} = \mathbb{C}^{H}{}_n + \frac{\Delta f_i}{1 - f_i}(\mathbb{C}_i - \mathbb{C}^{H}{}_n):\mathbb{A}_i{}^{D}$	
	$\mathbb{A}_i{}^{D} = [\mathbb{I} - \mathbb{S}^{H}{}_n:\mathbb{C}^{H}{}_n{}^{-1}:(\mathbb{C}^{H}{}_n - \mathbb{C}_i)]^{-1}$	
	Step 1:	
	$\mathbb{S}^{H} = \mathbb{S}, \mathbb{C}^{H}{}_n = \mathbb{C}_m$	
Four-phases	which is based on the three-phase model (Generalized Self-Consistent), associated with an analytical model, namely: "Composite Sphere Assemblage (CSA)" [22] or "Composite Cylinder Assemblage (CCA)" [33].	[21]
	$K^H = \left[K_m + \frac{f_i(K_i - K_m)(3K_m + 4G_m)}{3K_m + 4G_m + 3(1 - f_i)(K_i - K_m)}\right]$	
	$E_L^H = f_iE_i + f_mE_m + \frac{4f_if_m(\upsilon_i - \upsilon_m)^2G_m}{1 + \frac{3f_iG_m}{3K_m + G_m} + \frac{3f_mG_m}{3K_i + G_i}}$	
	$K_T^H = K_m + \frac{G_m}{3} + \frac{f_i}{\left[\frac{3}{3K_i + G_i - 3K_m - G_m}\right] + \left[\frac{3f_i}{3K_m + 4G_m}\right]}$	
	$G_L^H = \frac{(f_iG_i + f_mG_m + G_i)G_m}{f_mG_i + f_iG_m + G_m}$	
	$\upsilon_{LT}^H = f_iE_i + f_mE_m + \frac{3f_if_m(\upsilon_i - \upsilon_m)G_m\left[\frac{f_iG_m}{3K_m + G_m} + \frac{f_mG_m}{3K_i + G_i}\right]}{\left[\frac{3}{3K_i + G_i - 3K_m - G_m}\right] + \left[\frac{3f_i}{3K_m + 4G_m}\right]}$	
Multiphase	That bases its formulation on the famous study of double inclusion [38]. The model proposed [39], takes into consideration the assemblage of the Eshelby [28] tensor for all of the layers of existing materials in the modeling.	[39]
	$f_m + \sum_{1}^{n}(f_i + f_r) = 1$	
	$\mathbb{A}_i{}^{D} = I + \mathbb{S}_i:\Phi_i + \Delta\mathbb{S}:\Phi_r$	
	$\mathbb{A}_r{}^{D} = I + \mathbb{S}_r:\Phi_r + \frac{f_i}{f_r}\Delta\mathbb{S}:(\Phi_i - \Phi_r)$	
	$\Delta\mathbb{S} = \mathbb{S}_i - \mathbb{S}_r$	
	$\Phi_i = -\left[(\mathbb{S}_i + \mathbb{A}_i) + \Delta\mathbb{S}:\left(\mathbb{S}_i + \mathbb{A}_i - \frac{f_i}{f_r}\Delta\mathbb{S}\right):\left(\mathbb{S}_r + \mathbb{A}_r - \frac{f_i}{f_i}\Delta\mathbb{S}\right)^{-1}\right]^{-1}$	
	$\Phi_r = -\left[\Delta\mathbb{S} + (\mathbb{S}_i + \mathbb{A}_i):\left(\mathbb{S}_i + \mathbb{A}_i - \frac{f_i}{f_r}\Delta\mathbb{S}\right)^{-1}:\left(\mathbb{S}_r + \mathbb{A}_r - \frac{f_i}{f_i}\Delta\mathbb{S}\right)\right]^{-1}$	
	$\mathbb{A}_i = (\mathbb{C}_i - \mathbb{C}_m)^{-1}:\mathbb{C}_m$	
	$\mathbb{A}_r = (\mathbb{C}_r - \mathbb{C}_m)^{-1}:\mathbb{C}_m$	
	$\mathbb{C}^H = \mathbb{C}_m + \left[f_r(\mathbb{C}_r - \mathbb{C}_m):\mathbb{A}_r{}^{D} + f_i(\mathbb{C}_i - \mathbb{C}_m):\mathbb{A}_i{}^{D}\right]$	

Where $\mathbb{C}$ is the constitutive tensor for a linear elastic material, $\mathbb{S}$ is the Eshelby tensor, f is the volumetric fractions, $\mathbb{A}$ is the strain concentration tensor, $\mathbb{I}$ identity matrix, E is the modulus of elasticity, υ is the Poisson ratio, G the shear modulus and K the volumetric module, with the indices i, m, r, H, L, T respectively referring to inclusion, matrix, interphase, homogenized, longitudinal and transversal, the superscript D indicates dilute.

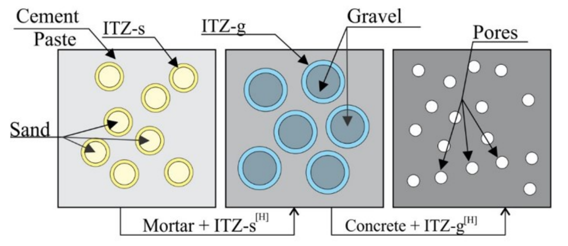
The Dilute Suspension model, although mentioned in Table 1, was not used in the micromechanical modeling of concrete due to its limitation when the volumetric fraction is high [37].

3 MULTI-SCALE HOMOGENIZATION OF CONCRETE

The procedure of homogenization adopted in this studied case considers the phases of construction of the material. To define the homogenized properties of concrete, the phases of the constitution of the composite (Figure 6) are considered in its meso-macroscale.



[a]



[b]

Figure 6: Three-level homogenization considering (without [a] /with [b]) interfacial transition zone and three- and multiple-phase models. Source: Author.

This way, each step receives as input a matrix and a random inclusion and provides as output the homogenized material. The elastic properties of the materials used for the composite construction are defined in Table 2. These parameters were quoted by Silva [18].

Table 2: Property of the composite phases (Experimental).

Material	Module of Elasticity (GPa)	Poisson ratio	Volumetric Fraction (%)
Cement Paste	21.34	0.25	15.40
Gravel	51.31	0.15	40.30
ITZ-1	10.17	0.30	2.30
Sand	77.60	0.15	26.90
ITZ-2	12.70	0.25	15.10
Concrete	34.50	-	-

Source: adapted from Li et al. [40].

In the first analysis, the composite is treated in a simplified way (Figure 6a), disregarding the presence of the transition zone, and the effective properties are calculated with two-phase models, in the second analysis, the four-phase and multiphase models including two more phases in the construction of the composite (Figure 6b). For both analyzes, in addition to the modulus of elasticity, the Poisson ratio and the estimated characteristic compressive strength of the concrete are evaluated.

Silva [41] explains that the longitudinal Young modulus (E_c) is a requirement for determining the characteristic strength of concrete (f_{ck}), being a parameter for several empirical models of strength prediction found in the literature. Some models can be seen in Table 3.

Table 3: Normative equations to estimate the modulus of elasticity of concrete.

Norm	Module of Elasticity estimate	Comments
NBR 6118 (2014)	$20 \leq f_{ck} \leq 50$ MPa $E_c = \alpha \cdot 5600\sqrt{f_{ck}}$ $55 \leq f_{ck} \leq 90$ MPa $E_c = 21.5 \cdot 10^3 \cdot \alpha \sqrt[3]{\frac{f_{ck}}{10} \cdot 1.25}$	$\alpha = 1.2$ (Basalt, dense limestone aggregates)
		$\alpha = 1.0$ (Quartzite aggregates)
		$\alpha = 0.9$ (Limestone aggregates)
ACI 3018 (2014)	$E_c = 5170\sqrt{f_{ck}}$	$\alpha = 0.7$ (Sandstone aggregates)
Fib Model Code (2010)	$12 \leq f_{ck} \leq 80$ MPa $E_c = 21.5 \cdot 10^3 \cdot \alpha \sqrt[3]{\frac{f_{ck}+8}{10}}$	$\alpha = 1.2$ (Basalt, dense limestone aggregates)
		$\alpha = 1.0$ (Quartzite aggregates)
		$\alpha = 0.9$ (Limestone aggregates)
		$\alpha = 0.7$ (Sandstone aggregates)
Eurocode 2 (2004)	$12 \leq f_{ck} \leq 90$ MPa $E_c = 23.1 \cdot 10^3 \cdot \alpha \left(\frac{f_{ck}+8}{10}\right)^{0.3}$	$\alpha = 1.2$ (Basalt, dense limestone aggregates)
		$\alpha = 1.0$ (Quartzite aggregates)
		$\alpha = 0.9$ (Limestone aggregates)
		$\alpha = 0.7$ (Sandstone aggregates)

In this way, the f_{ck} value can be found as a function of the longitudinal Young modulus, verifying the relative error between the homogenized concrete (with and without the ITZ) and the experimental value.

4 RESULTS AND DISCUSSIONS

To assess the calibration of micromechanical models with experimental results, the concept of relative error is used between the result obtained with the micromechanical analysis and the value obtained in the laboratory.

In the analysis of relative errors to obtain the effective elastic properties of the concrete, it was considered that the longitudinal Young modulus of 34.5 GPa, which was obtained experimentally by Li et al. [40], was considered.

One of the hypotheses raised would be the verification of limit models: models of Reuss, Voigt, and limits of Hashin. For this hypothesis, the construction of the composite without a transition zone was used (Figure 6a), with the corrections of the volumetric fractions for each of the three levels adopted in these two initials analyses shown in Table 4.

Table 4: Correction of volumetric fractions in the homogenization steps.

Level 4		Volumetric Fraction in Composite	Volumetric Fraction in Homogenization Level
Mortar homogenized	Cement paste	15.40%	36.41%
	Sand	26.90%	63.59%
	Total	42.30%	100.00%
Level 5		**Volumetric Fraction in Composite**	**Volumetric Fraction in Homogenization Level**
Concrete homogenized	Mortar homogenized	42.30%	48.79%
	Gravel	40.30%	51.21%
	Total	42.30%	100.00%
Level 6		**Volumetric Fraction in Composite**	**Volumetric Fraction in Homogenization Level**
Homogenized concrete adjusted	Concrete homogenized	100.00%	97.22%
	Pores	2.42%	2.78%
	Total	102.48%	100.00%

It should be noted that the errors for the analyzed analytical models are above 40% at the last level, which is not adequate. It is also observed that in the last homogenization step, the Reuss and Hashin [-] models are poorly conditioned since the pore modulus of elasticity is null and the relative error calculation would produce negative errors, which would not make physical sense (Table 5).

Continuing the modeling, two-phase models were used, disregarding the interfacial transition zone both in the sand and in the gravel, obtaining the following result in the homogenization steps (Table 6). When considering the two-phase numerical models in the homogenization process, a decrease in the concrete modeling error can be seen.

Table 5: Homogenization results for the limit models.

Models	Modulus of elasticity (GPa)			Error %		
	Level 4	Level 5	Level 6	Level 4	Level 5	Level 6
Reuss	39.596	44.559	-	14.770	26.156	-
Voigt	57.324	54.400	52.887	66.157	57.680	53.295
Hashin +	51.179	51.262	48.496	48.345	48.584	40.569
Hashin -	45.614	48.341	-	32.210	40.118	-
Concrete [40]	34.50					

Table 6: Homogenization results for the biphasic models.

Models	Modulus of elasticity (GPa)			Error %		
	Level 4	Level 5	Level 6	Level 4	Level 5	Level 6
Mori-Tanaka	45.614	48.341	45.671	32.215	40.118	32.379
Self-Consistent	49.304	50.290	47.436	42.909	45.768	37.496
Generalized Self-Consistent	46.144	48.624	45.937	33.751	40.938	33.325
Differential Scheme	46.772	48.923	46.981	35.571	41.806	36.177
Concrete [40]	34.50					

It can be seen that the two-phase homogenization models are not primarily responsible for

the high value of the relative error, with peaks of up to 37.496%, while the limit models had errors of 53.295%. This error is directly associated with the disregard of the interfacial transition zone in the composite construction and analysis process, even though the two-phase micromechanical models have limitations for concrete modeling.

The following analysis consists of modeling the concrete considering the interfacial transition zone, with models capable of evaluating more than two phases. The correction of volumetric fractions for these models can be seen in Table 7.

Table 7. Correction of volumetric fractions in the homogenization steps.

Level 4		Volumetric Fraction in Composite	Volumetric Fraction in Homogenization Level
Mortar homogenized + Interfacial Transition Zone of Sand	Sand	26.90%	46.86%
	ITZ-s	15.10%	26.31%
	Cement Paste	15.40%	26.83%
	Total	57.40%	100.00%
Level 5		**Volumetric Fraction in Composite**	**Volumetric Fraction in Homogenization Level**
Concrete homogenized + Interfacial Transition Zone of Gravel	Gravel	40.30%	40.30%
	ITZ-g	2.30%	2.30%
	Mortar homogenized + Interfacial Transition Zone of Sand	57.40%	57.40%
	Total	100.00%	100.00%
Level 6		**Volumetric Fraction in Composite**	**Volumetric Fraction in Homogenization Level**
Homogenized concrete adjusted	Concrete homogenized + Interfacial Transition Zone of Gravel	100.00%	97.64%
	Pores	2.42%	2.36%
	Total	102.48%	100.00%

In the last level of homogenization, the Mori-Tanaka model was used to correct the composite with pores. The obtained results reduced the error found by Li et al. [40] from 8% to below 5%, with the multiphase model reaching an insignificant error for the four-phase model, indicating a substantial gain when using a more robust homogenization model. Table 8 illustrates the decrease in error for each homogenization step.

As expected, more robust homogenization models combined with more experimented phases brought very satisfactory results. The error below 1% indicates that micromechanical models can accurately predict the homogenized properties of cementitious composites.

When evaluating the Poisson ratio homogenized for both the multiphase modeling (with ITZ and without ITZ), there were no significant differences, being in both models within the expected pattern Tables 9-10.

Table 8. Numerical results by homogenization steps.

Model	Modulus of elasticity (GPa)			Error %		
	Level 4	Level 5	Level 6	Level 4	Level 5	Level 6
Four-Phases	30.638	36.167	34.501	11.193	4.830	0.0031
Multiphase	32.101	37.774	36.302	6.952	9.488	4.441
Concrete [40]	34.50					

Table 9: Numerical results by homogenization steps for Poisson's ratio (without ITZ).

Models	Poisson ratio		
	Level 4	Level 5	Level 6
Mori-Tanaka	0.1997	0.1751	0.1759
Self-Consistent	0.1829	0.1671	0.1683
Generalized Self-Consistent	0.1942	0.1732	0.1741
Differential Scheme	0.182	0.172	0.173
NBR 6118	0.11 – 0.22		

Table 10. Numerical results by homogenization steps for Poisson's ratio (with ITZ).

Model	Poisson ratio		
	Level 4	Level 5	Level 6
Four-Phases	0.183	0.173	0.174
Multiphase	0.201	0.182	0.182
NBR 6118	0.11 – 0.22		

An estimate for the characteristic strength of concrete considered the values of Young's modulus found at Level 6 of the multiscale procedure, associated with two-phase models (without ITZ) Table 6 and multiple-phase models (with ITZ) Table 8. In the analysis, it was adopted a = 1 (Quartzite aggregates).

The estimated results for the characteristic strength of concrete, disregarding the interfacial transition zone, can be seen in Table 11.

Table 11: f_{ck} estimated using empirical models and homogenization (Level 6).

Models	*f_{ck} estimates (MPa)*				Error %			
	NBR 6118	ACI 3018	Fib Model Code	Eurocode 2	NBR 6118	ACI 3018	Fib Model Code	Eurocode 2
Mori-Tanaka	66.512	78.036	87,850	88.997	75.244	75.244	99.736	195.878
Self-Consistent	71.753	84.185	99.401	102.066	89.053	89.052	198.340	239.326
Generalized Self-Consistent	67.289	78.948	89.537	90.893	77.291	77.292	168.735	202.181
Differential Scheme	70.383	82.577	96.340	98.586	85.443	85.441	189.153	227.757
Concrete [40]	37.954	44.530	33.318	30.079	-	-	-	-

It is observed that there is an upward growth curve of the relative error, further demonstrating that it is not interesting to use two-phase models to estimate the strength of concrete. When using models that consider the interfacial transition zone, it is noted that the relative error also grows, but they are much smaller about two-phase models, which can be a support tool (Table 12).

Table 12: f_{ck} estimated using empirical models and homogenization (Level 6).

Models	*f_{ck} estimates (MPa)*				Error %			
	NBR 6118	ACI 3018	Fib Model Code	Eurocode 2	NBR 6118	ACI 3018	Fib Model Code	Eurocode 2
Four-Phases	37.956	44.533	33.321	30.083	0.005	0.007	0.009	0.013
Multiphase	42.022	49.303	40.136	37.122	10.718	10.719	20.463	23.415
Concrete [40]	37.954	44.530	33.318	30.079	-	-	-	-

It should be noted that the neglect of the transition zone directly influences the modeling of this type of concrete, and therefore, it should be included in the analysis. For conventional concretes, the use of two-phase models is not recommended, as it is not possible to introduce the interfacial transition zone in the analysis even if one wants to.

Increasing the levels of micromechanical multiscale modeling would be a hypothesis for use of two-phase models, but it could lead to problems of the inclusions not being spherical, or the matrix not being infinite which would go against the micromechanical formulation.

5 CONCLUSIONS

With conventional concrete, it is proven that two-phase models need to be well adjusted to being able to evaluate the homogenized properties of concrete [40] using essentially two-phase models with adaptations to include the interfacial transition zones in the analysis since the literature already confirms that their absence interferes drastically in the final result of the modeling. The errors obtained by Li et al. [40] were 8.7% using his strategy.

By modifying the strategy used by Li et al. [40] proposing a multiscale analysis with robust models of multiple phases, satisfactory results are effectively achieved, reducing the error to 4% in the multiphase model and zero when using the four-phase model.

This panorama indicates that in conventional concrete it is essential to evaluate the interfacial transition zone with more complex models, however a robust experimental apparatus to model this cementitious composite is still needed. Any neglected phase can significantly interfere in the micromechanical modeling and the possibility of removing any of its phases must be investigated on a case-by-case basis.

Every micromechanical multiscale procedure was applied to the meso and macro scale of concrete, however, every analysis methodology can be used on the microscale and also on smaller scales such as the nanoscale, always considering the definition of a representative volume element [37].

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