MICROMECHANICAL MODELING OF THE ELASTIC MODULUS OF THE ITZ OF CONCRETE

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ABSTRACT: The knowledge of the elastic modulus of concrete is important when it is applied as a structural material. The concrete has been assumed as a composite material of three phases, when the interfacial transition zone is considered as a phase of concrete. Concrete can be modeled and its elastic modulus is determined from the elastic properties of the components, as well as their respective volume fractions. The study was developed by analyzing the evolution of the elastic modulus of the ITZ over time, and these curves were obtained from experimental data. For modeling, we used the three phase sphere model [Chr79]. The properties of the interfacial transition zone are determined by inverse analysis. The presented results of the analysis with consideration of the time variation of elastic modulus of ITZ are shown to be agreement with the experimental data, whereas the analysis based on a two phase model, ignoring the ITZ, disagreed.

1 INTRODUCTION

The elastic modulus of the concrete is a necessary parameter in the structural analysis for the determination of the distributions of deformations and displacements, especially when structure design is based on elasticity parameters [Vil98].

According [Meh94], in the aggregate presence, the structure of the cement paste, in the great particle neighborhood, is commonly very different from the structure of the matrix of cement paste or mortar of the system. In fact, many aspects of the concrete behavior under stress can only be explained when the interface cement paste - aggregate it is dealt with as one third phase in the structure of the concrete.

Considering the concrete as a composite material of two phases, AITCIN & MEHTA (1990) cited in [Yan96] had demonstrated that the elastic modulus of the concrete is influenced by the elastic properties and volume fraction of aggregates.

The hypothesis of a two phase material is guaranteed as long as concrete satisfies the limits of Hashin-Shtrikman [Mon93], that they are derived from the linear elasticity theory for inclusions with arbitrary geometry. Experimental results show that the concrete does not satisfy to the reported limits. It’s followed that the concrete presents a third phase, the transition zone.

The micromechanics models already have been sufficiently used for the analysis of composite materials, presenting, in many cases, good results ([Li99a], [Li99b], [Zha97], [Yan96]).

Considering the concrete and the mortar as particulate materials, the application of micromechanics models for the description of its effective mechanical properties can provide good results and, consequently, constitutes a promising study.
[Yan98] analyzes the properties of concrete using micromechanical modeling, working with a three phase model and with estimates of the interface thickness, and its effective properties. For the thickness of 20 μm, the properties found are around 20% to 40% of the properties of the matrix of cement paste, whereas when the thickness is increased to 40 μm, this result to reach 50% to 70%.

[Lut97] and [Has02] refer to the elastic modulus of cement paste varying from 30% to 50% of the elastic modulus of the mortar. [Lee08] conducted a study comparing the elastic modulus of concrete with experimental results, assuming a variance between the elastic modulus of the ITZ and the cement paste of 30% to 70%. The reported results assume a specific date to take this variation, not taking into account that the properties of the ITZ, as well as mortar, vary over time, and that the relationship may no longer be constant.

Using the three phase sphere model, this work evaluates the influence of the consideration of the ITZ on the variation of the elastic modulus of concrete with time, from experimental results and numerical formulations.

2 AGGREGATES AND ITZ

The aggregates, essential components in the confection of the concrete, possess the peculiarity to occupy the biggest volume between mixture phases. The quality of the aggregates has direct influence on the properties of the concrete, and their properties can cause unsatisfactory performance, because they directly influence the behavior of the transition zone, although their compressive strength, in the majority of the cases, is not responsible for the rupture of the concrete.

According to [Li99b], the elastic modulus of concrete is influenced directly by maximum diameter of the coarse aggregate, respecting certain limits, where increases in the maximum diameter doesn’t cause significative variations in the elastic modulus of composite.

The observation of that the microcracks if initiates in the interface between the coarse aggregate and the paste and that, at rupture, the standard cracks include the interface, indicate to the importance of this part of the concrete [Nev97].

The structure of the interfacial transition zone, especially the void volume and microcracks, have great influence on the rigidity or the elastic modulus of the concrete.

In the composite material, the transition zone serves as a link between two constituents: the mortar matrix and the particles of the coarse aggregate. Especially in the cases where the individual constituents have high rigidity, the rigidity of the composite material can be low because of the voids and microcracks present in the transition zone, which do not allow energy transference [Meh94].
THREE PHASE SPHERE MODEL

According to [Li99a], for two-phase particulate-filled or fiber-reinforced composite materials, CHRISTENSEN & LO (1979) developed a three phase sphere model to estimate the effective bulk modulus and shear modulus. By overall evaluations, they concluded that this three-phase sphere model was more reasonable and reliable than other generally used models, such as the differential scheme and the Mori-Tanaka model, because the stress-strain field interactions between different inclusions were considered in this model.

The three phase sphere model has as hypothesis a sphere of composite material embedded in the infinite medium of unknown effective properties. For the determination of the elastic properties for this model, the sphere is composed of two phases, initially, matrix (domain $\Omega$) and inclusion (domain $\Omega_i$), that they are spheres of radii $b$ and $a$, respectively (Fig. 3.1). The volume fraction of inclusion is taken as a relation between the radii, being given by:

$$f_i = \left(\frac{a}{b}\right)^3$$

(3.1)

Fig. 3.1. Three phase sphere model.

On symmetrical spherical loading conditions, the strain on representative element volume is spherically symmetrical [Nem99], expressing the bulk modulus as:

$$\overline{K} = 1 + f_i \frac{(K_I - K_M)(3K_M + 4G_M)}{K_M(3K_M + 4G_M + 3(1-f_i)(K_I - K_M))}$$

(3.2)

where $K_M$ and $G_M$ are the bulk modulus and shear modulus for the matrix, while $K_I$ and $G_I$ are the respective modulus for the inclusion and $\overline{K}$ is the bulk modulus of composite. Equation 3.2 is valid for a three phase model [Nem99].

The three phase model considers the sphere embedded in an infinite and homogeneous medium (Fig. 3.1), submitted to uniform stress and strain applied very distant from the inclusion. These stress and strain are declared as $\sigma^\infty$ and $\varepsilon^\infty$, respectively. Are applied uniform traction and displacement conditions on the boundary to element volume representative.

Working in spherical coordinates, the boundary conditions can be written and the solution of the equilibrium equations for the stress and strain can be expressed according to LOVE (1927) cited in [Chr79].
For forced displacement on the boundary of the heterogeneous medium, ESHELBY (1956) cited in [Chr79] showed that the strain energy $U$, under applied displacement conditions, can be determined by:

$$U = U_0 - \frac{1}{2} \int_0^S \left( \sigma_i u_i^0 - \sigma_i^0 u_i \right) dS$$  \hspace{1cm} (3.3)

where $S_i$ is the surface of the inclusion, $U_0$ is the strain energy in the same medium when it contains no inclusion, $\sigma_i^0$ and $u_i^0$ are the tractions and displacements in the same medium when it contains no inclusion and $\sigma_i$ and $u_i$ are the corresponding quantities at the same point in the medium when it does contain the inclusion.

[Chr79] proved that $U = U_0$, rewriting eq. (3.3) as:

$$\frac{1}{2} \int_0^S \left( \sigma_i u_i^0 - \sigma_i^0 u_i \right) dS = 0 . \hspace{1cm} (3.4)$$

Applying the stress and strain in the radial and angular directions in (3.4), we have:

$$\frac{1}{2} \int_0^S \left( \sigma_r u_r + \tau_{r\phi} u_{\phi} + \tau_{\phi r} u_r - \sigma_r u_r^0 + \tau_{r\phi} u_{\phi}^0 \right) dS = 0 . \hspace{1cm} (3.5)$$

The conditions of shear at infinity for the problem are given by:

$$\begin{align*}
\sigma_r^0 &= 2G_D \sigma_2 \cos 2\phi \\
\tau_{r\phi}^0 &= 2G_D \tau_1 \cos \phi \cos 2\phi \\
\tau_{\phi r}^0 &= -2G_D \tau_1 \sin \phi \cos 2\phi \\
u_r^0 &= D_1 \tau_1 \cos 2\phi \\
u_{\phi}^0 &= -D_1 \tau_1 \sin 2\phi \\
\end{align*} \hspace{1cm} (3.6)$$

$$\begin{align*}
\sigma_r &= 2\sigma_2 \cos 2\phi \left\{ \frac{-3D_1 \lambda}{r^3} + 4D_1 + \frac{1}{r^5} \left( \frac{2(5 - 4v)D_4}{(1-2v)} \right) \right\} \\
\tau_{r\phi} &= \tau_1 \cos 2\phi \left\{ D_1 + \frac{8D_3}{r^5} + \frac{4(1+\tau)D_4}{(1-2v)^3} \right\} \hspace{1cm} . \hspace{1cm} (3.7) \\
\tau_{\phi r} &= \tau_1 \sin 2\phi \left\{ -2D_1 - \frac{16D_3}{r^5} + \frac{4(1+\tau)D_4}{(1-2v)^3} \right\} \\
\end{align*}$$

Evaluating eq. (3.5) for the effective shear modulus $\overline{G}$, we have:

$$A \left( \overline{G} \overline{G}_M \right)^2 + B \left( \overline{G} \overline{G}_M \right) + C = 0 \hspace{1cm} (3.8)$$

where $A$, $B$ and $C$ are listed in [Chr79].
4 METHODOLOGY

Some simplifications are required in connection with modeling, described below:

- The constituent phases and the effective composite material are assumed to be isotropic, within the linear elastic region.
- The aggregate is considered inert and maintains its elastic properties are constant over time.
- It is assumed that the interfacial transition zone (mortar - coarse aggregate) is a shell of constant thickness.
- The elastic modulus of the ITZ is assumed to be constant throughout its thickness.

The determination of the elastic modulus of the ITZ employed a numerical formulation based on the inversion of the equations 3.2 and 3.9 and the use of experimental results.

The analysis of the elastic modulus of concrete considering the interfacial transition zone is performed using two different approaches:

- Strategy 1: Effective Matrix (Mortar + ITZ) + Aggregate = Concrete. The elastic modulus of mortar + ITZ is obtained through a serie model. The serie model is described in [Meh06] as:
  \[
  \frac{1}{E} = \frac{f_1}{E_1} + \frac{f_2}{E_2},
  \] (4.1)

- Strategy 2: Effective Inclusion (Aggregate + ITZ) + Mortar = Concrete. The elastic modulus of aggregate + ITZ is obtained by the three phase sphere model.

For the experimental data, two concretes were mixed with compressive strengths of 35 MPa and 45 MPa, and the elastic modulus of concrete and mortar was tested at different ages, according to Brasilian Standard NBR 8522:2008, that describes the method for determining the elastic modulus of concrete.

The Poisson ratio of mortar were used as constants throughout the ages. To determine the bulk modulus and shear modulus is used the equation given by:

\[
E = \frac{9KG}{3K + G} = 2G(1 + \nu) = 3K(1 - 2\nu).
\] (4.2)

The mortars were obtained by separation of the coarse aggregates particles to the concrete produced.

5 MICROSTRUCTURE OF CONCRETE

For the concrete in this paper SEM-analysis was realized in order to assess the thickness of the ITZ layer and its evolution over time, relating the information found in the literature.

The tests were performed at the age of 28 days and younger than in order to verify, through identification of ITZ, if there was variation over time of its thickness.

[Dia01] observed that the higher porosity that characterizes the transition zone occurs within a minimum of 30 μm.
In Figure 5.1, microphotographs of samples of concrete studied at the age of 28 days are presented.

Fig. 5.1. Microphotographs of samples for concrete: (a) 35 MPa – 28 days, (b) 45 MPa – 28 days; (c) 35 MPa – 7 days; (d) 45 MPa – 17 days.

As a result of the evaluation of the images shown, it was observed that the thickness of ITZ is not much different between the two types of concrete, ranging from 30 µm to 100 µm, which reflects the information presented in the literature.

6 RESULTS E DISCUSSION

The micromechanical model for determining the modulus of ITZ and its influence on the concrete will be evaluated according to the strategies outlined in the methodology.

The elastic properties of the coarse aggregate are given in Table 6.1:

<table>
<thead>
<tr>
<th>Elastic properties for coarse aggregate.</th>
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<tbody>
<tr>
<td>Elastic modulus</td>
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<td>Poisson ratio</td>
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For the mortar, the value of the Poisson rate was assumed 0.17. The elastic modulus of mortar is shown in Figure 6.1.
Fig. 6.1. Variation of elastic modulus of concrete and mortar with time: (a) 35 MPa, (b) 45 MPa.

Figures 6.2a 6.2b presents the comparative analysis of experimental data with curves generated for the Hashin-Shtrikman bounds for concrete of 35 MPa and 45 MPa, respectively. The Hashin-Shtrikman bounds are used to characterize two phase composites and, if these limits are exceeded, denotes the presence of a third phase.

Fig. 6.2. Hashin-Shtrikman bounds to the concrete: (a) 35 MPa, (b) 45 MPa.

It is observed from Figure 6.2 that almost all experimental points lie outside the bounds proposed by Hashin-Shtrikman, which implies that the concrete material must be evaluated considering the ITZ as a phase.

Figure 6.3 shows the variation with time of the elastic modulus of the three phase sphere model and Mori-Tanaka model [Yan96], the latter for cylindrical and spherical aggregates, in the range from 3 days to 28 days.

The input data for analyzing the application of three phase sphere model and Mori-Tanaka model are the elastic modulus, Poisson ratio and volume fraction of phases. The elastic modulus of mortar was considered varying with time and Poisson's ratio of mortar was considered constant.
The data presented in Figure 6.3 were obtained experimentally (according to NBR 8522:2008) and the curves were fitted using polynomial models using average values (3 sample) for the ages, presented in some cases a reduction when evaluated over time. For the sample, were observed confidence intervals for each age to a significance level of 95%.

It is observed that the modeling using the three phase sphere and Mori-Tanaka models for determining the elastic modulus of concrete is not satisfactory, showing high errors for the fitted curve and the experimental data.

It follows that modeling through these models does not adequately represent the behavior of local concretes, because the same model be applied for determining the elastic modulus of concrete cited in [Sim95], where the modeling shows good results even without the consideration of the ITZ.

With the use of ITZ, the same is taken into account for determining of the elastic modulus of concrete with a constant Poisson ratio ($\nu = 0.2$) and varying the volume fraction of 8%, 10%, 12% and 15% in relation to the total mixture.

By applying the three phase sphere model, according to strategy 1, and applying the inversion of the equations as outlined in the methodology, can determine the elastic modulus of ITZ (Fig. 6.4). These curves were obtained by inversion of equations of three phase sphere model, considering the variation of volume fraction of the transition zone in relation to the total mixture.
Fig. 6.4. Evolution of the elastic modulus of ITZ with time.

The curves shown in Figure 6.4 shows the direct influence of the volume fraction of ITZ and, consequently, its thickness, on its elastic modulus. These values were obtained from the experimental data and show an evolution with time similar to the concrete and mortar.

Making use of results shown in Figure 6.4, the elastic modulus of concrete has been calculated by direct application to the model of the three phase sphere model according strategy 1.

In Figure 6.5 the variation of elastic modulus of concrete with time is shown.

Fig. 6.5. Evolution of the elastic modulus of concrete obtained with three phases sphere model (strategy 1).

It is observed in Figure 6.5 that for concrete of 45 MPa, the curves have good fit throughout the range examined. In contrast, the curve generated for concrete of 35 MPa showed good agreement for ages exceeding 15 days only. There is a slight tendency to better fit the experimental data curves with volume fraction of the transition zone between 10% and 12%, confirming data reported in [Dia01], [Ram96] and [Bon98].

According to the strategy 2, are presented curves of variation of the elastic modulus of concrete with time (Fig. 6.6). In this application, you first determined the modulus of elasticity of the association between aggregate and ITZ, and with this, it applies the model of three phase sphere for determining the modulus of the composite, leading to variation of modulus of mortar and ITZ with time.
The results show good estimate of the elastic modulus of concrete in relation to time by the methods applied, showing the importance of considering the transition zone in the analysis of concrete.

7 CONCLUSIONS

The paper includes the evaluation of the elastic modulus of the ITZ and its influence on concrete using micromechanical modeling, based on the three phase sphere model. This model has been tested and is considered one of the most accurate for evaluating the elastic modulus of concrete. [Bar08] and [Li99b] confirm the good accuracy of this model.

In the three phase sphere model, which despite the name is a two phase model, is performed a inversion of the main equations and it is determined the elastic modulus of the ITZ, presenting similar behavior the concrete.

In applying of micromechanical models to reproduce the behavior of concrete without the presence of ITZ, there is a great difference between numerical results and fitted curves of experimental data and, as seen on the limits of Hashin-Shtrikman, the ITZ should be considered for the modeling of concrete.

Data reported in [Lut97], [Has02] and [Lee08] show that the ratio of elastic modulus of the ITZ and cement paste varies between 0.3 and 0.5 and, according to the results, this ratio is confirmed to hold for the mortar and its transition zone.

The same conclusion can be obtained when analyzing the volume fraction of the transition zone with the reported in [Lee08], [Has02] and [Ram96], where the results in numerical analysis proved next to the experimental values for fractions ranging between 10% and 15%.

The curves presented in this study emphasize good estimates of modulus of elasticity of concrete at the consideration of the transition zone and the variation of its elastic modulus with time.
ACKNOWLEDGMENT

The authors thank CNPq – National Council of scientific and technological development.

REFERENCES


