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Finite element analysis of elastic property of concrete composites with ITZ

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Abstract. For better estimation of elastic property of concrete composites, the effect of Interfacial Transition Zone (ITZ) has been found to be significant. Numerical concrete composites models have been introduced using Finite Element Method (FEM), where ITZ is modeled as a thin shell surrounding aggregate. Therefore, difficulties arise from the mesh generation. In this study, a numerical concrete composites model in 3D based on FEM and random unit cell method is proposed to calculate elastic modulus of concrete composites with ITZ. The validity of the model has been verified by comparing the calculated elastic modulus with those obtained from other analytical and numerical models.

Keywords: elastic modulus; ITZ; numerical concrete composites model; finite element method; random unit cell; composite materials.

1. Introduction

The elastic modulus of concrete composites has been studied extensively. The primary phases in concrete or mortar are aggregate and matrix (bulk paste). Empirical expressions for the estimation of elastic modulus of mortar or concrete composites have been proposed (Hirsch 1962, Counto 1964, Lydon and Balendran 1986). In the field of composite mechanics, Hashin and Shtrikman (1963) have derived bounds for elastic modulus of two-phase materials. Christensen and Lo (1979) have obtained exact solutions for elastic modulus of a three-phase composite model consisting of inclusion, matrix and equivalent homogeneous medium. By assuming the concrete composites was a two-phase composite material, it was experimentally verified (Simeonov and Ahmad 1995) that the test fell below the lower Hashin and Shtrikman (H-S) bound (Hashin and Shtrikman 1963). Simeonov and Ahmad (1995) used H-S bounds and experimental data to investigate the elastic modulus of concrete composites. They concluded that concrete composites should be considered to be a three-phase composite instead of a two-phase one. Indeed, experiments have shown that the structure of the cement paste surrounding the aggregate differs from that of bulk cement paste. The phase in which the presence of the aggregates affects the properties of cement paste is taken as the Interfacial Transition Zone (ITZ) (Mehta and Monteiro 1993, Mindess 1989). The mechanical

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properties of concrete composites are controlled by the presence of ITZ. Therefore, a three-phase concrete is a composite material with aggregates as dispersed phase, ITZ as interphase, and cement paste as continuous phase or matrix. In addition to the influence of elastic modulus and volume fraction of aggregates and cement paste on the elastic modulus of concrete composites, it has been found by experiment that the elastic modulus of three-phase concrete is intimately related to the elastic modulus and volume fraction of ITZ (Simeonov and Ahmad 1995). The ITZ has a relatively more porous structure than the matrix one. The boundary between transition zone and matrix is hard to distinguish, and its stiffness may vary throughout its thickness. Because the volume fraction of ITZ is determined by the surface area of aggregate, while the surface area of aggregate is dependent on the maximum aggregate size and aggregate gradation, the volume fraction of ITZ and the corresponding elastic modulus of concrete composites should be closely related to the maximum aggregate size and aggregate gradation. It is estimated from experiments that the transition zone has lower stiffness than the bulk paste (Cohen *et al.* 1994). Thus, if the volume of the transition zone is not negligible, this may significantly affect the overall elastic modulus of mortar or concrete composites.

Many researchers have attempted to estimate the elastic modulus of concrete composites by analytical or numerical methods. In the simplest models, for the determination of elastic modulus of concrete composites without ITZ, empirical formulas have been obtained from experimental results. However, empirical formulas are often too simple to show the influence of various parameters and the use of a two-phase or three-phase model does not give insightful results because it does not consider ITZ. An analytical four-phase model which assumes that concrete composites are composed of aggregate, mortar matrix, ITZ and equivalent homogeneous medium has been introduced for the estimation of elastic modulus of concrete composites (Nadeau 2003, Hashin and Monteiro 2002, Ramesh *et al.* 1996, Garboczi 1997). ITZ is modeled as a thin shell surrounding aggregate. However, it is practically difficult to determine elastic modulus of concrete since ITZ is too thin. Numerical concrete composites models have been introduced using the conventional Finite Element Method. The difficulty to model concrete composites in 3D arises from the mesh generation. Conventional Finite Element Method allows only one material property to be assigned to each element. This makes mesh generation difficult because finite elements of ITZ are much smaller compared with the rest of the finite elements corresponding to aggregates and mortar matrix. Complicated interface between materials may cause that the shape of elements lose its convexity and lead to ill-conditioned stiffness matrix. In Lee and Park (2008), the authors propose a numerical concrete composites model which uses a three-phase model and finite element with material discontinuity for the determination of elastic modulus of concrete composites. The conventional numerical integration generally used in Finite Element Method is suited for an element consisting of a single material and not for an element composed of two or more materials. Adopting the numerical integration method which accurately computes the stiffness of finite elements with material discontinuity allows to describe ITZ influence on elastic modulus of concrete using uniform finite element mesh. The main concept of the numerical integration for an element with material discontinuity is given in Zohdi and Wriggers (2001). However, this method seems difficult to implement in finite element codes. Therefore, in this work, in order to avoid meshing difficulties and to provide a powerful tool for fast calculation of elastic modulus of concrete composites, we propose to use random unit cell Finite Element Method. The random unit cells generated allows us to investigate the effects of ITZ in the unit cell model. A study has been conducted with random unit cell method in order to evaluate the effect of ITZ phase and the bounds of the method for the prediction of elastic modulus in concrete composites. Results will be compared with other approaches.

2. Numerical concrete composites model

Analytical and semi analytical models have been developed to evaluate the material properties of distributed particles composites based on the homogenization techniques. They are often reduced to specific cases. Therefore, numerical models seem to be a well suited approach to describe the behavior of these materials, because there is no restriction on the geometry, on the material properties, and on the number of phases in the composite. One approach to designing new composites is using predictive Finite Element Method (FEM) to highlight the effects of changes in material properties on the elastic mechanical properties of the composite. Young's modulus E is an important mechanical property that may be calculated by a variety of methods. In order to obtain realistic macroscopic behavior predictions of new composites by the computational means, 3D numerical simulation of statistically representative micro-heterogeneous material samples is unavoidable.

In the study of composites, periodic 2D unit cells (Marus 2004), 3D single-particle and two-particle unit cells finite element models have been used in the predictive analysis of elastic properties of composites (Llorca *et al.* 2000). However, all periodic unit cells are based on the assumption that the composite is made up of a repeated structure. The randomness of particle arrangement in composites is neglected. Recently, some random unit cells have been developed to model distributed particles composites (Gusev 1997, Bohm *et al.* 2002, Segurado and Llorca 2003, Kari *et al.* 2007, Sun *et al.* 2007). Effective properties of randomly distributed spherical particles composites using Random Sequential Adsorption (RSA) algorithm have been assessed and compared with different analytical methods. In this work, a numerical homogenization approach is based on the FEM and random unit cells. It allows the extension of the composites with arbitrary geometrical inclusion configurations, providing a powerful tool for fast calculation of their properties. RSA algorithm is used to generate the 3D Representative Volume Element (RVE) models of randomly distributed particles.

2.1 Numerical generation of random unit cell model

The elastic properties of the composite are obtained by the finite element analysis of a periodic cubic unit cell (RVE) of volume L^3 containing a random distribution of non-overlapping particles. The final particle generation has to be statistically isotropic (all directions in the unit cell are equivalent) and in addition it should be suitable for finite element discretization. Both conditions can be fulfilled using RSA algorithm to generate the coordinates of the particle centers (Rintoul and Torquato 1997). According to this method and for spherical particle of diameter D, the inclusion center positions are generated randomly and sequentially. Particle i is accepted if the center coordinates verify the following conditions:

- The center distance between spherical particle i and all other particles, which are previously accepted $j = 1, \ldots, i-1$ have to exceed a minimum value $(2r + s_1)$, where r is the particle radius and s_1 is the minimum distance between neighboring spherical particles, imposed by the practical limitations for creating an adequate finite element mesh.
- The distance between particle surface and the cubic RVE surfaces and corners have to exceed a minimum value s_2 in order to avoid the presence of distorted finite elements during meshing.
- If the surface of the spherical particle i cuts any of the cubic RVE surfaces, this condition has to be checked with the spherical volumes on the opposite surfaces because the microstructure of the composite is periodic.

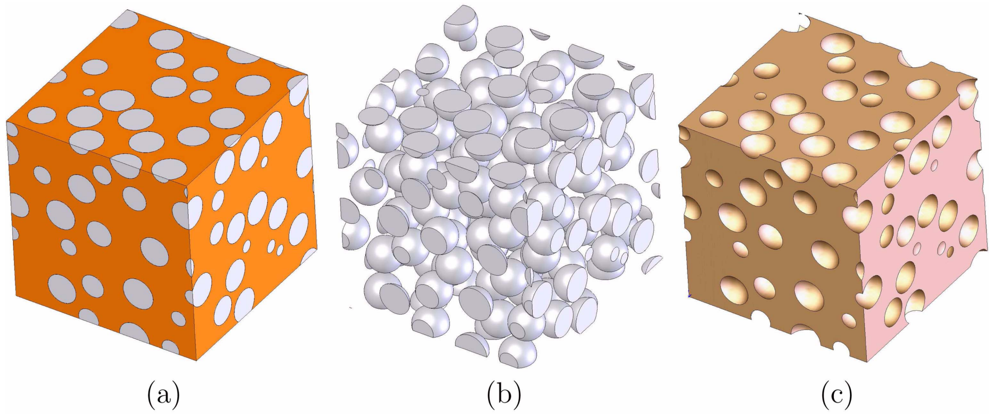


Fig. 1 Unit cell model generated (RVE) for 30% volume fraction of spherical aggregates, $L = 12$ mm, $D = 2$ mm, $s_1 = 0.05r$, $s_2 = 0.05r$: (a) Complete unit cell, (b) Aggregates, (c) Matrix

RSA algorithm with the combination of the above conditions was used to generate RVE models of the studied composite up to desired volume fractions of aggregates. The main idea of the method is to find a globally homogeneous medium equivalent to the original composite. In the numerical homogenization technique, the common approach to model the macroscopic properties of particle composites is to create the RVE that should capture the major features of the underlying microstructure. Random unit cell model generated is shown in Fig. 1.

2.2 Random unit cell finite element analysis

All finite element calculations were made with the commercial FE package COSMOSWORKS. The matrix and the particles were meshed with 10 node-tetrahedral elements with full integration. Perfect bond is assumed across particle/matrix interfaces. Uniaxial loading is employed and can be either iso-displacement or iso-stress type. The iso-displacement loading predicts the upper bound of

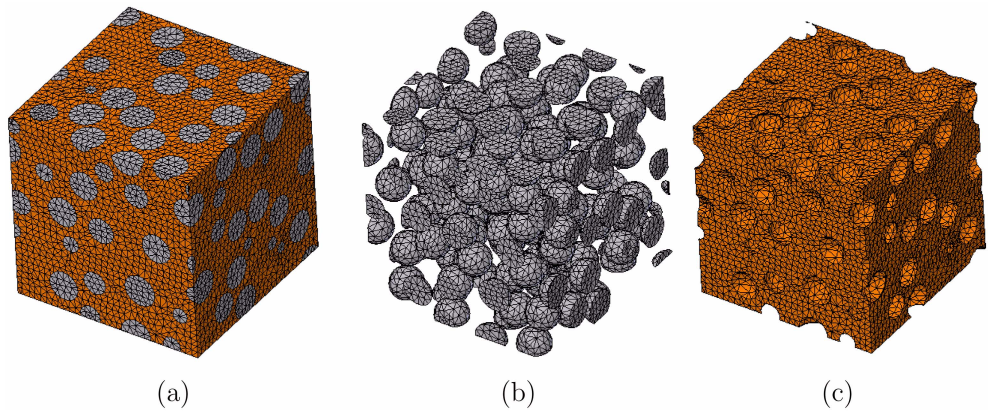


Fig. 2 Finite element models generated for 30% volume fraction of spherical aggre-gates, $L = 12$ mm, D = 2 mm, $s_1 = 0.05r$, $s_2 = 0.05r$: (a) Complete meshed RVE, (b) Meshed aggregates, (c) Meshed matrix

Young's modulus, while iso-stress loading predicts the practical lower bound of Young's modulus E. For iso-displacement loading, a small strain of 1% is used. For iso-stress loading, a uniform compressive pressure is applied. The finite element models of the random unit cell are shown in Fig. 2.

A study has been conducted in Abdelmoumen *et al.* (2007) to evaluate the effect of various material and numerical parameters of the random unit cell method for the prediction of Young's modulus of concrete composites.

The method to generate a unit cell with randomly distributed particles is based on the following: if a large piece of composite is divided into equal halves, both halves will maintain the mechanical properties of the original. If the process is continued many times, eventually a critical size will be reached, below which the properties of the original composite will not be retained. The critical size of the random unit cell is determined as the smallest size which is representative of the overall composite. With the random unit cell method, the critical size of the cubic unit cell of volume L^3 containing a random distribution of non-overlapping particles is generally regarded as a volume L^3 of a heterogeneous material that is sufficiently large to be statistically representative of the composite (Kanit *et al.* 2003). Whereas in many analytical methods, in the case of random unit cell method, one must take care of the minimum size of the RVE which is required to give appropriate effective material properties of a macroscopic composite structure. From these results (Abdelmoumen *et al.* 2007), it can be observed that it is sufficient to assume the critical size of RVE as $L/D \geq 5$. This value enables us to obtain a very small difference in Young's modulus and deviations around the mean value for different unit cells generated. Moreover, with $L/D \geq 5$ the difference in Young's modulus between iso-displacement and iso-stress loading is very small. Therefore, in the following, we will assume iso-displacement loading and $L/D \geq 5$ in order to generate and to load random unit cells. In Abdelmoumen *et al*. (2007), homogeneity and isotropy of generated cells have been examined. The tests have shown that the method used to generate unit cells gives homogeneous and isotropic cells for a wide range of ratio L/D. They have confirmed the choice to assume the size of RVE as $L/D \geq 5$. Moreover, the results have shown that elastic modulus is not influenced (less than 1%) by the size, the gradation and the shape of aggregates (Abdelmoumen *et al*. 2007).

2.3 Numerical concrete composites model without ITZ

Before evaluating elastic modulus of concrete composites with ITZ, we propose to consider concrete as a two-phase composite in order to show that the proposed method correlates with previous analytical and experimental results.

Firstly, a comparison is made with a method based on Mori-Tanaka theory and Eshelby's method (Yang and Huang 1996) and published experimental data (Anson and Newman 1966). The Young's modulus of cement paste and aggregates are $E_m = 28.3$ GPa and $E_a = 69$ GPa respectively. The Poisson's ratio of cement paste and aggregates are $\nu_m = 0.22$ and $\nu_a = 0.21$ respectively. For the numerical concrete composites model considered in this work, a constant diameter $D = 2$ mm is chosen for spherical aggregates and $L/D = 6$ is assumed. For the different approaches, Fig. 3 shows the Young's modulus E of concrete obtained with different aggregate volume fractions V_a. From Fig. 3, we can see a better correlation between experimental results and the proposed numerical concrete composites model.

Secondly, a comparison is made with the values obtained by a numerical concrete model proposed in Lee and Park (2008) and Christensen-Lo's model (three-phase composite sphere model) (Christensen and Lo 1979) to verify the effectiveness of the proposed approach. The Young's

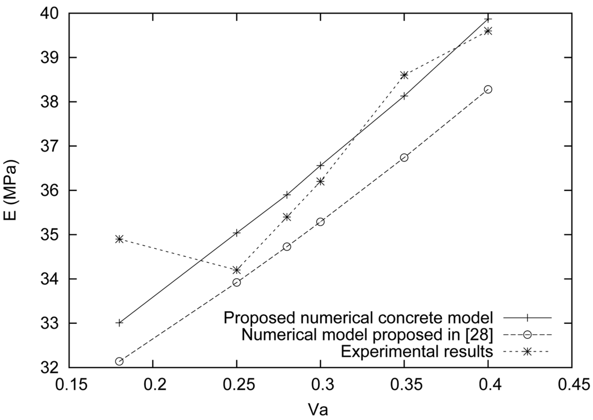


Fig. 3 Two-phase concrete composite: comparison with previous analytical and experimental results

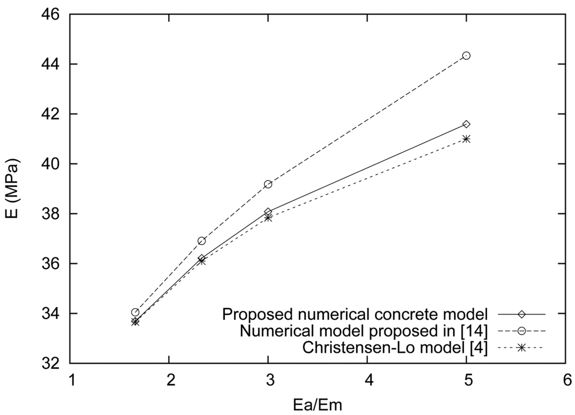


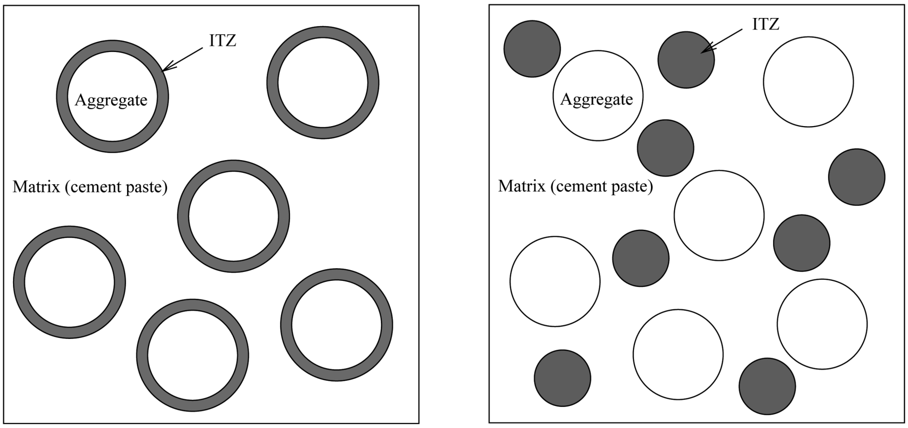
Fig. 4 Two-phase concrete composite: comparison with previous analytical and numerical results

modulus of cement paste is $E_m = 30$ GPa and Poisson's ratio of cement paste and aggregates are $\nu_m = 0.2$ and $\nu_a = 0.2$ respectively. Volume fraction of aggregates is set to $V_a = 23\%$. For the numerical concrete composites model considered in this work, a constant diameter $D = 2$ mm is chosen for spherical aggregates and $L/D = 6$ is assumed. For the different approaches, Fig. 4 shows the Young's modulus E of concrete obtained with different ratios (E_a/E_m). The values calculated by the proposed numerical concrete composites model agree well with the values by Christensen-Lo's model, as shown in Fig. 4.

3. Numerical concrete composites model with ITZ

The assumptions used in this work are detailed below.

- The elastic modulus of constituent phases and also those of resulting composites are assumed to be isotropic.
- The aggregate inclusions are assumed to be spherical. In concrete composites, the aggregates usually have randomly varying shapes. The sharp corners of the aggregates induce stress concentrations that initiate micro-crack propagation. The overall stiffness of a composite unlike strength is an average macroscopic property, and is less sensitive to the shape of the inclusion.
- Elastic properties of concrete composites depend not only on the elastic properties of aggregate, ITZ and cement paste but also on the aggregate size, ITZ layer thickness. It is noted that the elastic properties of ITZ vary through its thickness. In this work, however, ITZ is assumed to be uniform layer for simplicity and we consider the same aggregate size.
- The elastic properties of ITZ can be estimated from existing studies. For example, in Lutz *et al.* (1997), Young's modulus of ITZ is about 30-50% less than the Young's modulus of cement paste. It has been shown that in actual concrete composites, although the thickness of ITZ layer depends on factors such as water/cement ratio, it seems to be independent of the size of inclusions (Scrivener and Nemati 1996). Therefore, it is reasonable to assume the thickness of ITZ layer to be constant. A number of researchers have experimentally investigated ITZ layer thickness and elastic modulus. They found that the average thickness of ITZ layer in typical concrete is about 50 μm.



(a)− First approach (b)− Second approach

Fig. 5 Numerical concrete composites model with ITZ (conceptual illustrations of 3D models)

- We assume that there is no overlap of ITZ layers between neighboring aggregates.

We propose to compute elastic modulus of concrete composites using the random unit cell Finite Element Method. In the first approach, ITZ is described by a thin layer surrounding aggregate (Fig. 5a). In order to avoid meshing difficulties, we assume that the thickness of ITZ layer is 100 μm. In the second approach, ITZ is described by a distinct phase of spherical inclusions equal to the volume fraction of a thin layer adopted in the first approach (Fig. 5b). While the first approach is closer to reality than the second, it is difficult to carry out finite element models with ITZ layer less than 100 μm. Indeed, the mesh generation is difficult because finite elements of ITZ are much smaller compared with the rest of the finite elements. This problem can lead to ill-conditioned stiffness matrix. The second approach avoids meshing problems and allows to describe concrete composites with very thin thickness of ITZ (less than 100 μm). Indeed, this numerical approach has the advantages of the rapid mesh generation of 3D concrete models with uniform finite elements and the elimination of elements distorsion. The results of the first approach with the thickness of ITZ layer equal to 100 μm are considered as the reference. The estimations of elastic moduli calculated by the second approach are compared with the results of the first approach This comparison allows us to investigate the suitability of the second approach.

The numerical concrete composites model is considered as a three-phase material composed of matrix, ITZ and aggregates. Let E_m, E_{itz}, E_a and $\nu_m = \nu_{itz} = \nu_a$ as their elastic modulus and Poisson's ratios, respectively. Volume fraction of aggregates is set to $V_a = 20\%$, $L/D = 6$ and a constant diameter $D = 2$ mm is chosen for spherical aggregates. For the first approach, the thickness of ITZ is $t_{itz} = 100$ μm. Therefore, the volume fraction of ITZ $V_{itz} = 6.62\%$ is given by

$$V_{itz} = \left[\frac{(D/2 + t_{itz})^3}{(D/2)^3} - 1 \right] V_a \tag{1}$$

For the second approach, we assume a constant diameter $D_{itz} = 2$ mm for the spherical ITZ phase and a volume fraction of ITZ $V_{itz} = 6.62\%$.

For the analysis, we have adopted dimensionless mechanical properties. As seen above, ITZ is

Table 1 Elastic modulus of concrete composites calculated with the proposed numerical models

$E_m = 100$, $V_a = 20\%$, $V_{itz} = 6.62\%$, $L/D = 6$, $D = 2$ mm					
First approach $t_{itz} = 100$ μm			Second approach $D_{itz} = 2$ mm		
$E_a = 2$ $E_a = 0.02E_m$	$E_{itz} = 0.3E_m$ $E_{itz} = 0.5E_m$ $E_{itz} = 0.7E_m$	$E_1 = 61.06$ $E_1 = 63.14$ $E_1 = 65.06$	$E_a = 2$ $E_a = 0.02E_m$	$E_{itz} = 0.3E_m$ $E_{itz} = 0.5E_m$ $E_{itz} = 0.7E_m$	$E_2 = 61.90$ $E_2 = 63.76$ $E_2 = 65.18$
$E_a = 10$ $E_a = 0.1E_m$	$E_{itz} = 0.3E_m$ $E_{itz} = 0.5E_m$ $E_{itz} = 0.7E_m$	$E_1 = 65.86$ $E_1 = 67.86$ $E_1 = 69.66$	$E_a = 10$ $E_a = 0.1E_m$	$E_{itz} = 0.3E_m$ $E_{itz} = 0.5E_m$ $E_{itz} = 0.7E_m$	$E_2 = 66.21$ $E_2 = 68.17$ $E_2 = 69.66$
$E_a = 20$ $E_a = 0.2E_m$	$E_{itz} = 0.3E_m$ $E_{itz} = 0.5E_m$ $E_{itz} = 0.7E_m$	$E_1 = 70.71$ $E_1 = 72.79$ $E_1 = 74.54$	$E_a = 20$ $E_a = 0.2E_m$	$E_{itz} = 0.3E_m$ $E_{itz} = 0.5E_m$ $E_{itz} = 0.7E_m$	$E_2 = 71.09$ $E_2 = 72.88$ $E_2 = 74.45$
$E_a = 50$ $E_a = 0.5E_m$	$E_{itz} = 0.3E_m$ $E_{itz} = 0.5E_m$ $E_{itz} = 0.7E_m$	$E_1 = 80.94$ $E_1 = 83.65$ $E_1 = 85.56$	$E_a = 50$ $E_a = 0.5E_m$	$E_{itz} = 0.3E_m$ $E_{itz} = 0.5E_m$ $E_{itz} = 0.7E_m$	$E_2 = 81.44$ $E_2 = 83.72$ $E_2 = 85.46$
$E_a = 80$ $E_a = 0.8E_m$	$E_{itz} = 0.3E_m$ $E_{itz} = 0.5E_m$ $E_{itz} = 0.7E_m$	$E_1 = 87.67$ $E_1 = 91.12$ $E_1 = 93.34$	$E_a = 80$ $E_a = 0.8E_m$	$E_{itz} = 0.3E_m$ $E_{itz} = 0.5E_m$ $E_{itz} = 0.7E_m$	$E_2 = 89.09$ $E_2 = 91.55$ $E_2 = 93.45$
$E_a = 100$ $E_a = E_m$	$E_{itz} = 0.3E_m$ $E_{itz} = 0.5E_m$ $E_{itz} = 0.7E_m$	$E_1 = 91.00$ $E_1 = 95.00$ $E_1 = 97.44$	$E_a = 100$ $E_a = E_m$	$E_{itz} = 0.3E_m$ $E_{itz} = 0.5E_m$ $E_{itz} = 0.7E_m$	$E_2 = 93.17$ $E_2 = 95.88$ $E_2 = 97.71$
$E_a = 120$ $E_a = 1.2E_m$	$E_{itz} = 0.3E_m$ $E_{itz} = 1.2E_m$ $E_{itz} = 0.7E_m$	$E_1 = 93.77$ $E_1 = 98.23$ $E_1 = 100.90$	$E_a = 120$ $E_a = 1.2E_m$	$E_{itz} = 0.3E_m$ $E_{itz} = 0.5E_m$ $E_{itz} = 0.7E_m$	$E_2 = 96.66$ $E_2 = 99.31$ $E_2 = 101.36$
$E_a = 150$ $E_a = 1.5E_m$	$E_{itz} = 0.3E_m$ $E_{itz} = 0.5E_m$ $E_{itz} = 0.7E_m$	$E_1 = 97.13$ $E_1 = 102.23$ $E_1 = 105.23$	$E_a = 150$ $E_a = 1.5E_m$	$E_{itz} = 0.3E_m$ $E_{itz} = 0.5E_m$ $E_{itz} = 0.7E_m$	$E_2 = 101.09$ $E_2 = 103.83$ $E_2 = 105.97$
$E_a = 200$ $E_a = 2E_m$	$E_{itz} = 0.3E_m$ $E_{itz} = 0.5E_m$ $E_{itz} = 0.7E_m$	$E_1 = 101.31$ $E_1 = 107.33$ $E_1 = 110.80$	$E_a = 200$ $E_a = 2E_m$	$E_{itz} = 0.3E_m$ $E_{itz} = 0.5E_m$ $E_{itz} = 0.7E_m$	$E_2 = 106.88$ $E_2 = 109.77$ $E_2 = 112.02$
$E_a = 500$ $E_a = 5E_m$	$E_{itz} = 0.3E_m$ $E_{itz} = 0.5E_m$ $E_{itz} = 0.7E_m$	$E_1 = 112.36$ $E_1 = 121.43$ $E_1 = 126.71$	$E_a = 500$ $E_a = 5E_m$	$E_{itz} = 0.3E_m$ $E_{itz} = 0.5E_m$ $E_{itz} = 0.7E_m$	$E_2 = 124.18$ $E_2 = 127.50$ $E_2 = 130.11$
$E_a = 1000$ $E_a = 10E_m$	$E_{itz} = 0.3E_m$ $E_{itz} = 0.5E_m$ $E_{itz} = 0.7E_m$	$E_1 = 117.84$ $E_1 = 128.82$ $E_1 = 135.32$	$E_a = 1000$ $E_a = 10E_m$	$E_{itz} = 0.3E_m$ $E_{itz} = 0.5E_m$ $E_{itz} = 0.7E_m$	$E_2 = 134.23$ $E_2 = 137.79$ $E_2 = 140.62$
$E_a = 5000$ $E_a = 50E_m$	$E_{itz} = 0.3E_m$ $E_{itz} = 0.5E_m$ $E_{itz} = 0.7E_m$	$E_1 = 123.47$ $E_1 = 136.72$ $E_1 = 144.80$	$E_a = 5000$ $E_a = 50E_m$	$E_{itz} = 0.3E_m$ $E_{itz} = 0.5E_m$ $E_{itz} = 0.7E_m$	$E_2 = 146.11$ $E_2 = 148.33$ $E_2 = 153.06$

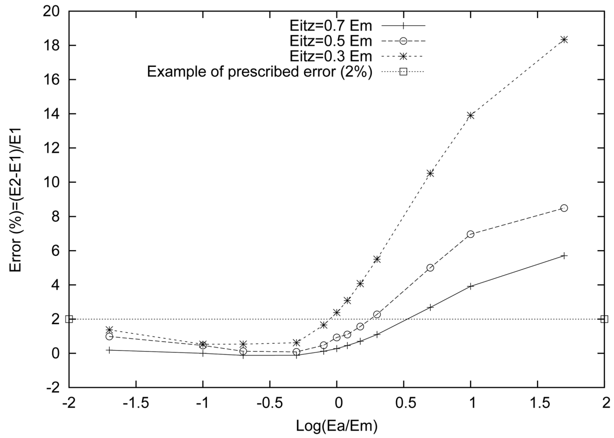


Fig. 6 Evolution of the error between E_1 (first approach) and E_2 (second approach)

assumed to be a uniform phase with a ratio (E_{itz}/E_m) within the range of 30%–70%. In order to study a large number of possible cement-based composites, the elastic modulus E of concrete is calculated with a ratio (E_a/E_m) within the range of 2%–5000%. Table 1 shows the elastic modulus of concrete calculated with the different approaches. Fig. 6 gives the evolution of the error between the first approach considered as much closer to reality (reference) and the second approach versus the ratio $log(E_a/E_m)$ for different ratios (E_{itz}/E_m). From these curves, we observe the following facts. The elastic modulus of concrete is affected significantly by the ratio (E_{itz}/E_m). The difference between the approaches decreases when the ratio (E_{itz}/E_m) increases. If the aggregate is softer than the matrix (cement paste), the error is always smaller than 2% whatever the ratio (E_{itz}/E_m). If the aggregate is harder than the matrix, the error increases with the increase of the ratio (E_a/E_m) and with the decrease of the ratio (E_{itz}/E_m). Therefore, if we prescribed for example an error less than 2% by using the second approach, we can define the following bounds (Fig. 6)

$$\begin{cases} \dfrac{E_{itz}}{E_m} = 0.7 \text{ then } 0.02 \le \dfrac{E_a}{E_m} \le 5 \\ \dfrac{E_{itz}}{E_m} = 0.5 \text{ then } 0.02 \le \dfrac{E_a}{E_m} \le 2 \\ \dfrac{E_{itz}}{E_m} = 0.3 \text{ then } 0.02 \le \dfrac{E_a}{E_m} \le 1 \end{cases} \tag{2}$$

The bounds of the model defined above, enables the second method to be used for the elastic modulus estimation of a large number of possible cement-based composites. In the following, we propose to compare the results of the second approach with results obtained in the literature.

4. Comparison with analytical solutions

In Ramesh *et al.* (1996), a four-phase composite model consisting of aggregate, matrix, ITZ and equivalent homogeneous medium is used to model a three-phase composite such as concrete or mortar. This composite spheres model is an extension of the two-phase composite spheres model

(Hashin and Shtrikman 1963). Analytical solutions for the elastic modulus of the four-phase composite model are presented. The aggregate with ITZ and matrix can be viewed as a heterogeneous inclusion that is embedded in the infinite equivalent homogeneous medium. The assumptions used in analytical solutions of this model are detailed below.

- The elastic modulus of constituent phases and also those of resulting composites are assumed to be isotropic.
- The aggregate inclusions are assumed to be spherical.
- The derivation of analytical solutions uses linear theory of elasticity. The effects of porosity in transition zone, aggregate and matrix are not considered.
- The thickness of transition zone is assumed to be constant. Also, its elastic modulus is taken to be constant thickness.

The elastic modulus computed from a four-phase composite model is compared with the elastic modulus computed from the second approach presented in this work. The volume fraction of ITZ is assumed as 10%, E_{itz} value is taken as 0.5 E_m. $E_m = 19.17$ GPa, $E_{itz} = 9.59$ GPa and $\nu_m = \nu_{itz} = 0.26$. Mechanical characteristics of the aggregates are given in Table 2. For the numerical concrete composites model considered in this work, constant diameters $D = 2$ mm and $D_{itz} = 2$ mm are respectively chosen for spherical aggregates and the spherical ITZ phase. Table 3 shows the elastic modulus of concrete composites derived from the analytical model (Ramesh *et al.* 1996) and the second approach of the numerical concrete composites model. The comparison of elastic modulus is given in Fig. 7. Moreover, we have studied the influence of V_a on the error between the numerical approach and the analytical approach versus the ratio $log\ (E_a/E_m)$ (Fig. 7). Firstly, for $(E_{itz}/E_m) = 0.5$ considered in this example, we find again the bounds of the numerical model defined by Eq. (2). Indeed, if we prescribed for example an error less than 2% by using the second approach of the numerical concrete composites model, we obtain $0.86 \leq (E_a/E_m) \leq 2$. In Ramesh *et al.* (1996), (E_a/E_m) less than 0.86 is not considered. However, we can assume that for softer aggregates, the bounds of the numerical model (2) should be found again. Secondly, from Fig. 7 we observe a very low influence of V_a on the error versus $log\ (E_a/E_m)$. This remark allows us to extend the applicability and the bounds of the numerical model for different values of V_a.

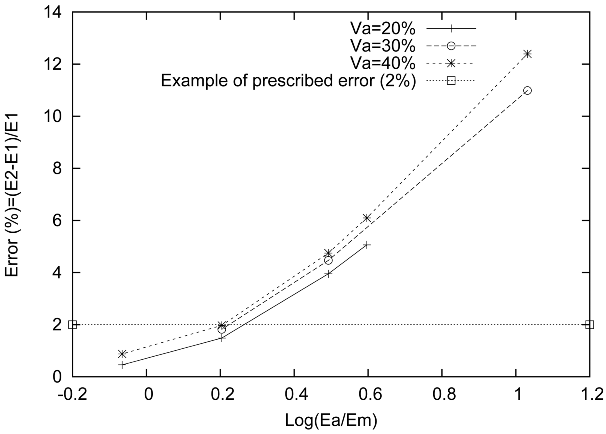


Fig. 7 Evolution of the error between E_1 (analytical model) and E_2 (second ap-proach of the numerical model). $E_{itz} = 0.5E_m$

Table 2 Mechanical characteristics of the aggregates

Aggregate type	E_a (GPa)	ν_a
Steel	206	0.3
Sand	75.8	0.15
Gravel	59.6	0.15
Limestone	30.7	0.15
Lead	16.6	0.45

Table 3 Elastic modulus of concrete composites calculated with analytical and numerical models

V_{itz} = 10%, E_{itz} = 0.5 E_m, E_m = 19.17 GPa, $\nu_m = \nu_{itz}$ = 0.26					
Analytical model (Ramesh *et al.* 1996)			Numerical model (second approach) D = 2 mm, D_{itz} = 2 mm, L/D=6		
V_a = 20%	Sand	E_1 = 22.12	V_a = 20%	Sand	E_2 = 23.24
	Gravel	E_1 = 21.51		Gravel	E_2 = 22.36
	Limestone	E_1 = 19.49		Limestone	E_2 =19.78
	Lead	E_1 = 17.55		Lead	E_2 =17.63
V_a = 30%	Steel	E_1 = 28.13	V_a = 30%	Steel	E_2 =31.22
	Gravel	E_1 = 23.73		Gravel	E_2 =24.79
	Limestone	E_1 = 20.35		Limestone	E_2 =20.72
V_a = 40%	Steel	E_1 = 33.66	V_a = 40%	Steel	E_2 =37.83
	Sand	E_1 = 28.06		Sand	E_2 =29.77
	Gravel	E_1 = 26.34		Gravel	E_2 =27.59
	Limestone	E_1 = 21.31		Limestone	E_2 =21.73
	Lead	E_1 = 17.11		Lead	E_2 =17.26

5. Comparison with another numerical model

In Lee and Park (2008), the authors propose a numerical concrete model which uses a three-phase model and finite element with material discontinuity for the determination of elastic modulus of concrete. The conventional numerical integration generally used in Finite Element Method is suited for an element consisting of a single material and not for an element composed of two or more materials. Adopting the numerical integration method which accurately computes the stiffness of finite elements with material discontinuity allows to describe ITZ influence on elastic modulus of concrete using uniform finite element mesh. The main concept of the numerical integration for an element with material discontinuity is given in Zohdi amd Wriggers (2001).

The elastic modulus computed from the numerical concrete model with material discontinuity is compared with the elastic modulus computed from the second approach of the proposed model. The volume fraction of ITZ is within the range 1% − 7% and the ratio (E_{itz}/E_m) within the range 0.3 − 0.7. V_a = 39.2%, E_m = 37.7 GPa, E_a = 58.8 GPa and $\nu_m = \nu_{itz} = \nu_a$ = 0.3. For the numerical concrete composites model considered in this work, constant diameters D = 2 mm and D_{itz} = 2 mm are respectively chosen for spherical aggregates and the spherical ITZ phase. The comparison of elastic modulus computed from the numerical concrete model with material discontinuity and those computed from numerical concrete composites model with the second approach is given in Table 4. This comparison allows us to verify the bounds of the numerical model defined by Eq. (2). Moreover, we have studied the influence of V_{itz} on the error between the numerical approaches versus the ratio (E_{itz}/E_m) (Fig. 8). We have observed a low influence of V_{itz} on the error for different values of the ratio (E_{itz}/E_m). As defined in Eq. (2), for (E_a/E_m)=1.56 considered in this example, the error is always less than 2% for V_{itz} within the range 1% − 7 %. This remark allows us to extend the applicability and the bounds of the numerical model for different values of V_{itz}.

Table 4 Elastic modulus of concrete composites calculated with two numerical models

V_a = 39.2%, E_m = 37.7 GPa, E_a = 58.8 GPa, $\nu_m = \nu_{itz} = \nu_a = 0.3$					
Numerical model with material discontinuity (Lee and Park 2008)			Numerical model (second approach) D = 2 mm, D_{itz} = 2 mm, L/D = 6		
V_{itz} = 1%	$E_{itz} = 0.3E_m$	E_1 = 44.17	V_{itz} = 1%	$E_{itz} = 0.3E_m$	E_2 = 44.22
	$E_{itz} = 0.5E_m$	E_1 = 44.27		$E_{itz} = 0.5E_m$	E_2 = 44.39
	$E_{itz} = 0.7E_m$	E_1 = 44.31		$E_{itz} = 0.7E_m$	E_2 = 44.52
V_{itz} = 2%	$E_{itz} = 0.3E_m$	E_1 = 43.86	V_{itz} = 2%	$E_{itz} = 0.3E_m$	E_2 = 43.78
	$E_{itz} = 0.5E_m$	E_1 = 43.96		$E_{itz} = 0.5E_m$	E_2 = 44.11
	$E_{itz} = 0.7E_m$	E_1 = 44.10		$E_{itz} = 0.7E_m$	E_2 = 44.38
V_{itz} = 3%	$E_{itz} = 0.3E_m$	E_1 = 43.44	V_{itz} = 3%	$E_{itz} = 0.3E_m$	E_2 = 43.32
	$E_{itz} = 0.5E_m$	E_1 = 43.67		$E_{itz} = 0.5E_m$	E_2 = 43.83
	$E_{itz} = 0.7E_m$	E_1 = 43.90		$E_{itz} = 0.7E_m$	E_2 = 44.23
V_{itz} = 4%	$E_{itz} = 0.3E_m$	E_1 = 43.08	V_{itz} = 4%	$E_{itz} = 0.3E_m$	E_2 = 42.87
	$E_{itz} = 0.5E_m$	E_1 = 43.39		$E_{itz} = 0.5E_m$	E_2 = 43.54
	$E_{itz} = 0.7E_m$	E_1 = 43.68		$E_{itz} = 0.7E_m$	E_2 = 44.06
V_{itz} = 7%	$E_{itz} = 0.3E_m$	E_1 = 42.01	V_{itz} = 7%	$E_{itz} = 0.3E_m$	E_2 = 41.61
	$E_{itz} = 0.5E_m$	E_1 = 42.53		$E_{itz} = 0.5E_m$	E_2 = 42.75
	$E_{itz} = 0.7E_m$	E_1 = 43.04		$E_{itz} = 0.7E_m$	E_2 = 43.64

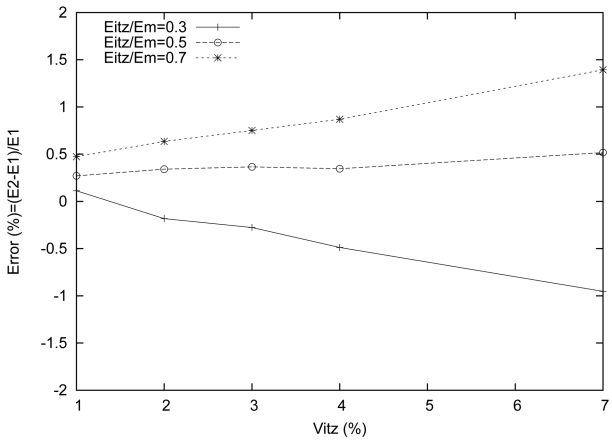


Fig. 8 Evolution of the error between E_1 (numerical model with material discontinuity) and E_2 (second approach of the numerical model). (E_a/E_m) = 1.56

6. Conclusions

A numerical concrete composites model has been proposed for better estimation of elastic modulus of concrete composites with ITZ. The numerical model adopts the Finite Element Method and random unit cell method. In spite of the fact that the proposed approach does not consider ITZ as a thin layer of matrix material surrounding each aggregate, the estimations of elastic modulus of concrete composites are in good agreement with results given in the literature. The bounds of the model enable the method to be used for elastic modulus estimation of a large number of possible cement-based composites. For the determination of concrete composites elastic modulus, the method provides a powerful tool for fast calculation of 3D numerical concrete composites model, avoids meshing problems and allows to describe concrete composites with very thin thickness of ITZ.

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