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A numerical investigation of the effect of the interfacial zone in concrete mixtures under uniaxial compression The case of the dilute limit

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Abstract

A two-dimensional numerical investigation concerning the effects of the interfacial transition zone (ITZ) on the mechanical behavior of concrete is presented in this paper. The ITZ lies between the cement paste and the aggregates. Considering elastic two-dimensional models of the cement paste, the aggregate material and the ITZ, which is modeled as a thin band around each grain of aggregate, the response of the composite material was calculated using the finite element method. A parametric analysis was conducted for different model geometries as well as varying model parameters for the dilute limit, i.e. when the aggregate volume fraction is very small. Results indicate that the maximum tensile stresses which could lead to the development of microcracks, as well as larger displacements, tend to develop mainly in the ITZ. The distribution of stresses and displacements along appropriate sections of these models are also presented.

Keywords: Finite element analysis; Microstructure; Interfacial transition zone; Concrete

1. Introduction

Over the recent years, there has been increasing interest in the numerical study and analysis of the microstructure and the properties of cement-based materials, mainly due to the decrease of computing cost and the wide availability of fast computers. A variety of models, both numerical and analytical, have been proposed by a number of scientists [1–8] in order to cast some light on the mechanical performance of these materials. A concrete mixture commonly involves two main phases: the aggregate phase and the cement paste phase. The aggregate phase consists of irregularly shaped particles characterized by a wide size distribution from millimeters to centimeters, i.e. sand and rock fragments. The cement paste phase fills the matrix between the particles and, during this process, a third phase, the interfacial zone, is developed. Typically, the sand size ranges up to a few millimeters, while rock size ranges up to 30 or 40 mm. Theoretical analysis as well as experimental results have revealed the existence of a third phase in these concrete mixtures, that of the interfacial zone, which exists around aggregate particles [1,4–6,16].

The term "interfacial", "interstitial" or "transition zone" (ITZ) in a concrete mixture, is used to define a region up to 50 μm wide, located between the aggregate particles and the bulk of the cement paste around the aggregate. Because the average aggregate diameter is much larger than the average cement grain diameter, the aggregates on the average will appear locally flat to the cement grains, so the ITZ thickness will depend on the median size of the cement grains and not on the aggregate size [4]. This zone contains less cement and is characterized by larger pores (and higher porosity) than the bulk cement paste. Furthermore, this region was found to contain large crystals of calcium hydroxide [4,9]. Due to the aforementioned features, the ITZ is considered to be the weak link in a concrete composite with respect to mechanical performance and durability [10].

Focusing on the properties of the ITZ, many researchers have attempted to quantify the influence of the ITZ on the mechanical behavior of a concrete composite. Analytical formulas to calculate the ITZ volume have been proposed [4]. Mathematical analysis of the diffusivity and the conductivity of the ITZ at the dilute limit (i.e. when the

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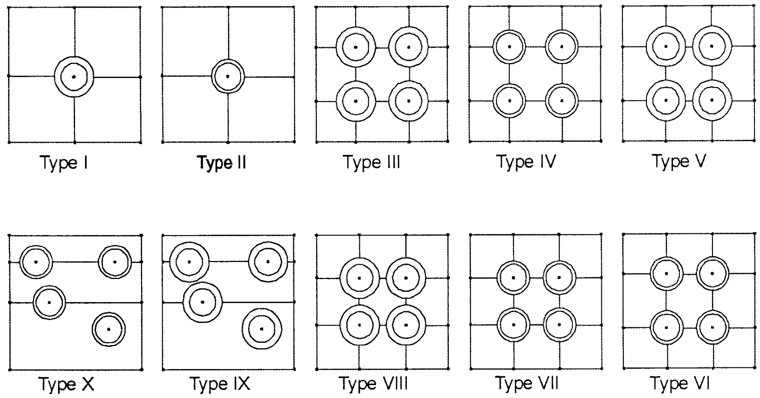


Fig. 1. Model types.

inclusion phase is present at a very small volume fraction) have been conducted [6], and material properties have been estimated using simulation, as well as experimental and analytical techniques [1,5,10–12,16]. In a recent study [5], the effects of the elastic moduli of the ITZ were studied by creating mono-size circles for sand grains of different diameters. A 20-μm thick ITZ surrounded each of the particles. The Poisson's ratio of the ITZ was set to 0.3, while Young's modulus of the ITZ was varied between 20% and 500% of the bulk cement paste modulus. The overall composite modulus was estimated via parametric analysis. The effect of the surface of the ITZ was also evaluated [5].

As already established, the behavior of the ITZ is directly related to the mechanical performance of the concrete composite mixture. It is also accepted that the properties of the ITZ are gradient and not uniform. For simplicity, however, most researchers assume uniform ITZ properties. However, the properties of the ITZ cannot be directly evaluated. In the present study, the behavior of the ITZ and its impact on the mechanical performance of a concrete mixture were studied for a normalized two-dimensional case study using finite element method techniques. A parametric study was conducted in an attempt to simulate the mechanism that generates stress concentrations that will eventually lead to specimen failure. This method is also utilized in applied homogenization problems in the numerical analysis of composite materials [13].

2. Formulation of the problem

In order to numerically evaluate the behavior of the ITZ under loading, several two-dimensional simulation models of the microstructure of the concrete mixture were developed and subsequently modeled using the finite element method.

Initially, a cubic concrete specimen was considered with dimensions equal to $10 \times 10 \times 10$ cm. These dimensions correspond to the specimens that were produced and tested in the laboratory of the Greek Center for Cement Research and correspond to the minimum dimensions for a specimen tested under uniaxial compression. In order to effectively model and analyze the effects of the ITZ, the dimensions of the problem were reduced, and thus, a 2-mm cubic element at the center of the cubic specimen was considered. Subsequently, the three-dimensional problem was reduced to two-dimensional by considering a plane strain analysis for the upper right quadrant (1×1 mm) of this square element, which was modeled considering the symmetry with respect to the X and Y coordinate axes of this element. In the following sections, the assumptions and/or simplifications regarding geometry, material models, and boundary conditions that were utilized in order to design and analyze these two-dimensional models are presented.

3. Model geometry

For these models, it was assumed that the aggregate phase consists only of circular sand particles with a constant diameter equal to 0.2 mm. The ITZ is modeled by a ring, which surrounds each sand particle. The width of this ring varies from 25 to 50 μm. The properties of the ITZ are considered uniform. The models consist of either one or four grains of sand surrounded by the respective ITZ bands, while the remaining space is occupied by cement paste. According to the number of sand particles modeled and their location in each model (distance between the particles and the boundaries of the model), five different types of models were defined. By considering

Table 1
Model types and location of the grains of sand

Distance between grains (mm)		Model type	
Horizontal	Vertical	ITZ 50 μm	ITZ 25 μm
0.40	0.40	III	IV
0.35	0.40	V	VI
0.35	0.35	VII	VIII
Random	Random	IX	X

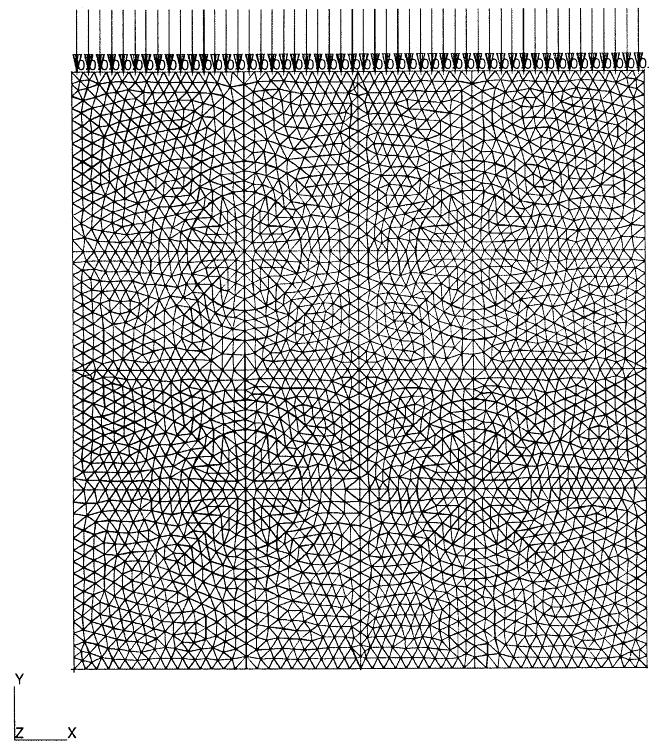


Fig. 2. Four-grain computer model.

two cases for the thickness of the ITZ, i.e. 25 and 50 μm, 10 model types were defined. Types I and II correspond to the models which include one grain of sand located at the center of the element. Types III to X correspond to models, which include four grains of sand (Fig. 1). The positioning of the four grains of sand in these models is presented in Table 1.

It should be noted that the decision to model an elementary portion of an actual specimen and to model the aggregate phase as sand grains in the dilute limit was mainly dictated by the difficulties encountered when trying to create a realistic representation of a random distribution of variable size particles in a two-dimensional specimen model, given the practical restrictions of a finite element mesh.

4. Loading and boundary conditions

Each model was subjected to a uniaxial compressive load of 27 N/mm^2. This load was developed using stress–strain data from laboratory measurements, which were adjusted to model geometry. The boundary conditions, which reflect the symmetry of the *X*- and *Y*-axes, were as follows:

- The left edge of each model was permitted to slide along the *Y*-axis.
- The lower edge of each model was permitted to slide along the *X*-axis.
- The intersection point of the left and the lower edge was fixed (i.e. movement or rotation was not allowed in any direction).

Table 2
Mechanical properties of the cement phases

Cement paste		Aggregates		ITZ	
E_{cp} (N/mm^2)	ν_{cp}	E_a (N/mm^2)	ν_a	E_{iz} (N/mm^2)	ν_{iz}
8000	0.22	80 000	0.20	2000–4000–6000–8000	0.20

5. Material model assumption

All three phases of the concrete mixture were modeled in the linear elastic region. The values of Young's modulus

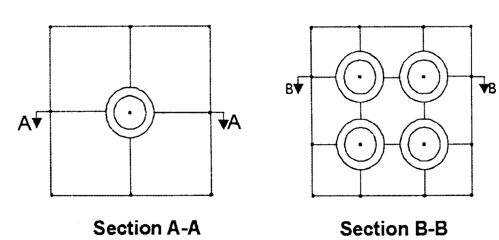
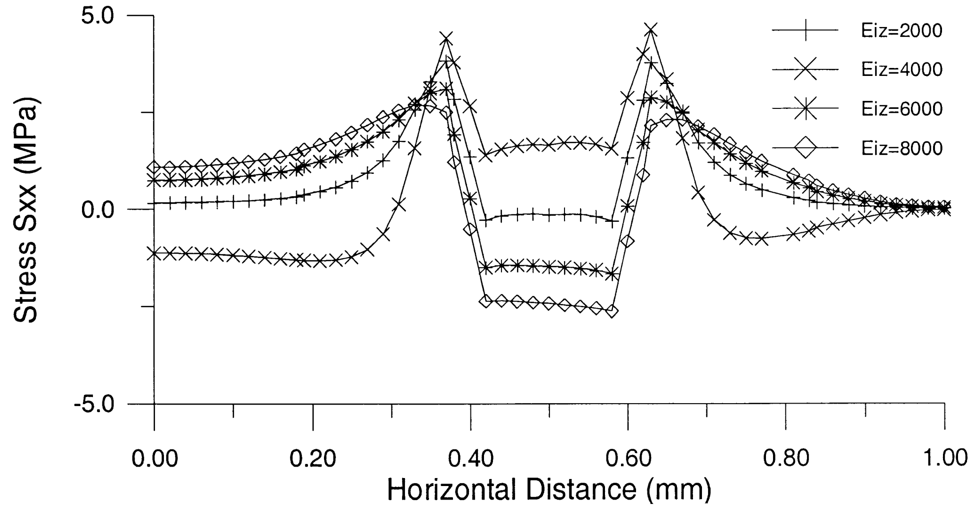
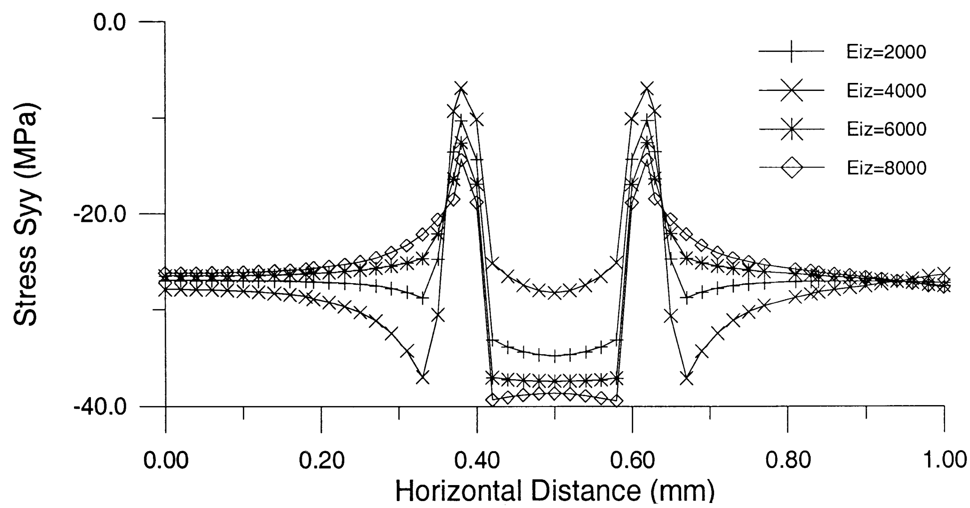
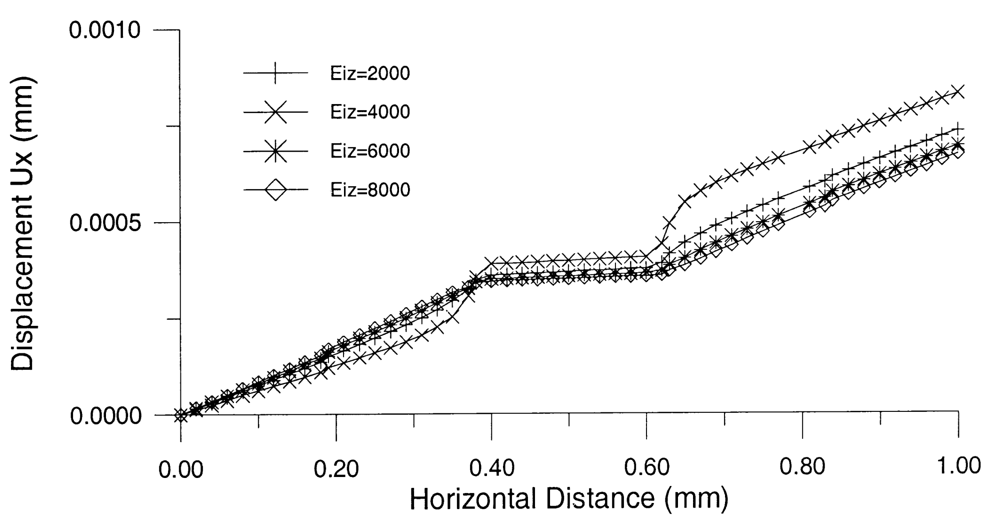


Fig. 3. Cross-sections used for presenting the distribution of stress and displacement in each model.


5.0
0.0
-5.0
Stress Sxx (MPa)
0.00
0.20
0.40
0.60
0.80
1.00
Horizontal Distance (mm)
Eiz=2000
Eiz=4000
Eiz=6000
Eiz=8000


0.0
-20.0
-40.0
Stress Syy (MPa)
0.00
0.20
0.40
0.60
0.80
1.00
Horizontal Distance (mm)
Eiz=2000
Eiz=4000
Eiz=6000
Eiz=8000


0.0010
0.0005
0.0000
Displacement Ux (mm)
0.00
0.20
0.40
0.60
0.80
1.00
Horizontal Distance (mm)
Eiz=2000
Eiz=4000
Eiz=6000
Eiz=8000

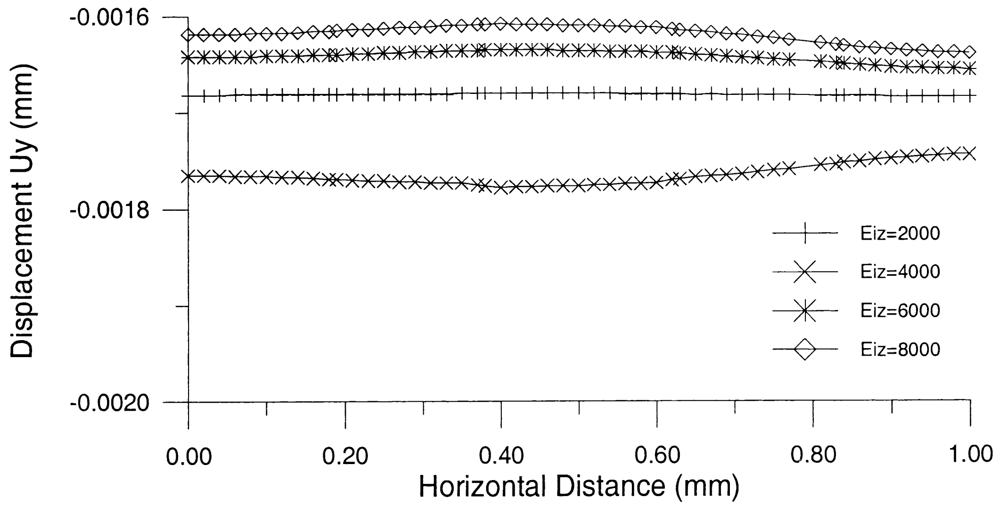


Fig. 4. (a) Stress Sxx for section A–A for model Type I. (b) Stress Syy for section A–A for model Type I. (c) Horizontal displacement for section A–A for model Type I. (d) Vertical displacement for section A–A for model Type I.

and Poisson's ratio, for each of these phases as used in this study, are given in Table 2. The values for the cement paste and the aggregates were drawn from a study by Simeonov and Ahmad [14] and correspond to a concrete with a water–cement ratio equal to 0.60. The values for the cement paste have also been verified from tests conducted in the laboratory of the Greek Center for Cement Research [15].

The values for the ITZ are the unknown quantity. For that reason, a parametric analysis was introduced, where the Poisson's ratio was defined at 0.20 and Young's modulus was varied from a minimum of 2000 N/mm^2 to a maximum 8000 N/mm^2 with intervals of 2000 N/mm^2. Thus, the ratio E_{iz}/E_{cp} varied between 0.25 and 1. It should be noted that experiments have shown that the ITZ demonstrates elastoplastic behavior [10]. However, for reasons of simplicity and time needed for calculations, this was not taken into consideration in this study. Based on the above information, 40 numerical models were created, four for each geometry type, which correspond to varying Young's modulus for the ITZ.

Each model was discretized using triangular elements with three nodes per element. Each node was allowed 3 *dof* (displacements along the *X*- and *Y*-axis and rotation about the *Z*-axis). In the initial phases of this research, various mesh sizes were tested. Results were similar for all models where the ITZ was sufficiently discretized. Models employing a few thousand elements were typically selected based on the time needed for calculations, since once a certain limit was exceeded for the particular workstation, heavy memory paging occurred and solution time increased. It should also be noted that the ITZ was discretized with similar density as the surrounding material. Fig. 2 shows a four-grain model with 3110 nodes and 6018 elements. This was a typical size for the meshes that were created for all 10 types of models. The appropriate boundary/loading conditions and material properties were defined for each model and were subsequently analyzed using the MSC-NASTRAN software system.

6. Results

The stresses and the displacements for each node were extracted from the static analysis of each model. In order to compare the results from different models, stress and displacement components were plotted along pre-selected cross-sections of the models. A few characteristic diagrams, corresponding to cross-sections A–A and B–B (Fig. 3), are presented, as an aid to the evaluation of the behavior of the ITZ in this analysis.

The distribution of both the stress and displacement components (vertical and horizontal), which correspond to a Type I model (the width of the ITZ is taken equal to 50 μm) are presented in Fig. 4a–d. High horizontal and vertical stresses are evident on both sides of the ITZ for all variations of the elastic modulus of the ITZ. It is worth noting that the highest stress concentrations were presented for E_{iz} = 4000 N/mm^2 although this was expected to occur at the minimum E_{iz} value employed (Fig. 4a and b). Fig. 5a and b presents the distribution of vertical and horizontal stress components for a Type III model. Higher stresses are evident within the particles, while lower stresses are developed between the aggregate particles. The effects of the ITZ are not clearly presented due to the low resolution along the profiles.

7. Discussion of results and conclusions

From the results of this analysis, several observations can be made regarding the behavior of a concrete mixture

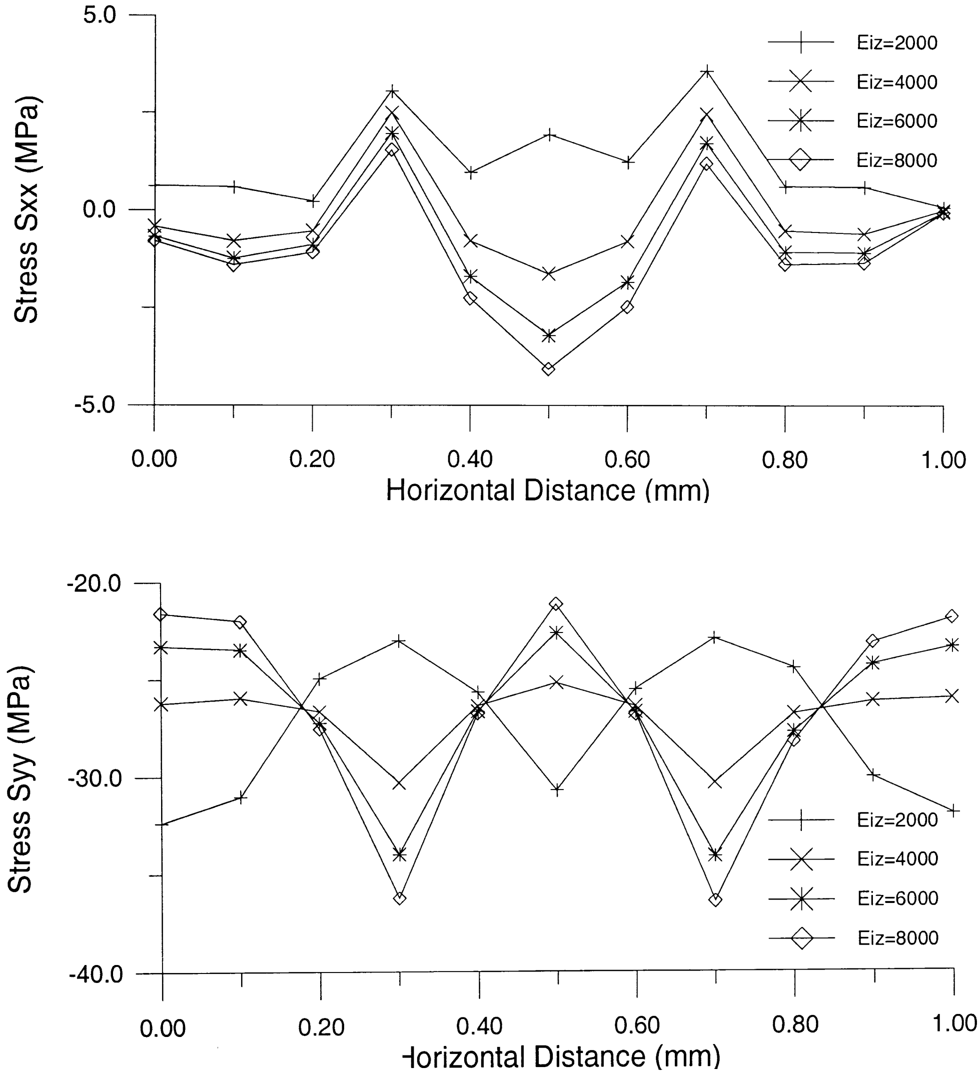


Fig. 5. (a) Stress Sxx for section B–B for model Type III. (b) Stress Syy for section B–B for model Type III.

under uniaxial compression, particularly regarding the concentration and distribution of horizontal (Sxx) and vertical (Syy) stresses as well as the variation of the horizontal (Ux) and vertical (Uy) displacements. It should be emphasized that this analysis pertains to the dilute limit and it is concentrated on the effect of the size and properties of the ITZ on the stresses that may lead to or promote failure of a concrete specimen. Furthermore, the ITZ is considered of uniform shape and type which reflects the average properties of this zone on the overall mechanical behavior of a block. However, since in the dilute limit there are much less aggregate grains than in actual specimens, these observations are accurate to the local level, but are more qualitative than quantitative when addressing the effect to the whole specimen.

Regarding the stress component Sxx, a concentration of tensile stresses in the ITZ region of the models is noted, and at the same time, a propagation of these stresses inside the sand particles is evident. These stresses achieve their maximum values when the modulus of elasticity of the ITZ is set at its minimum value (E_{iz}/E_{cp} = 0.25). These stress concentrations diminish as the modulus of elasticity of the ITZ increases. The same remarks are appropriate for both widths of the ITZ that were evaluated.

Regarding the distribution of stress component Syy, a constant value is achieved inside the sand particles with values in the order of the imposed one. The above statement is also true for the cement paste region, especially near the edges of the models. In the region of the ITZ, the Syy significantly decreases in value.

The values for the horizontal displacement values, Ux, seem to increase in a linear manner towards the outer edge of the models. The ITZ region experiences greater displacements compared to the cement paste region. The Ux displacements appear to be constant along the sand particles.

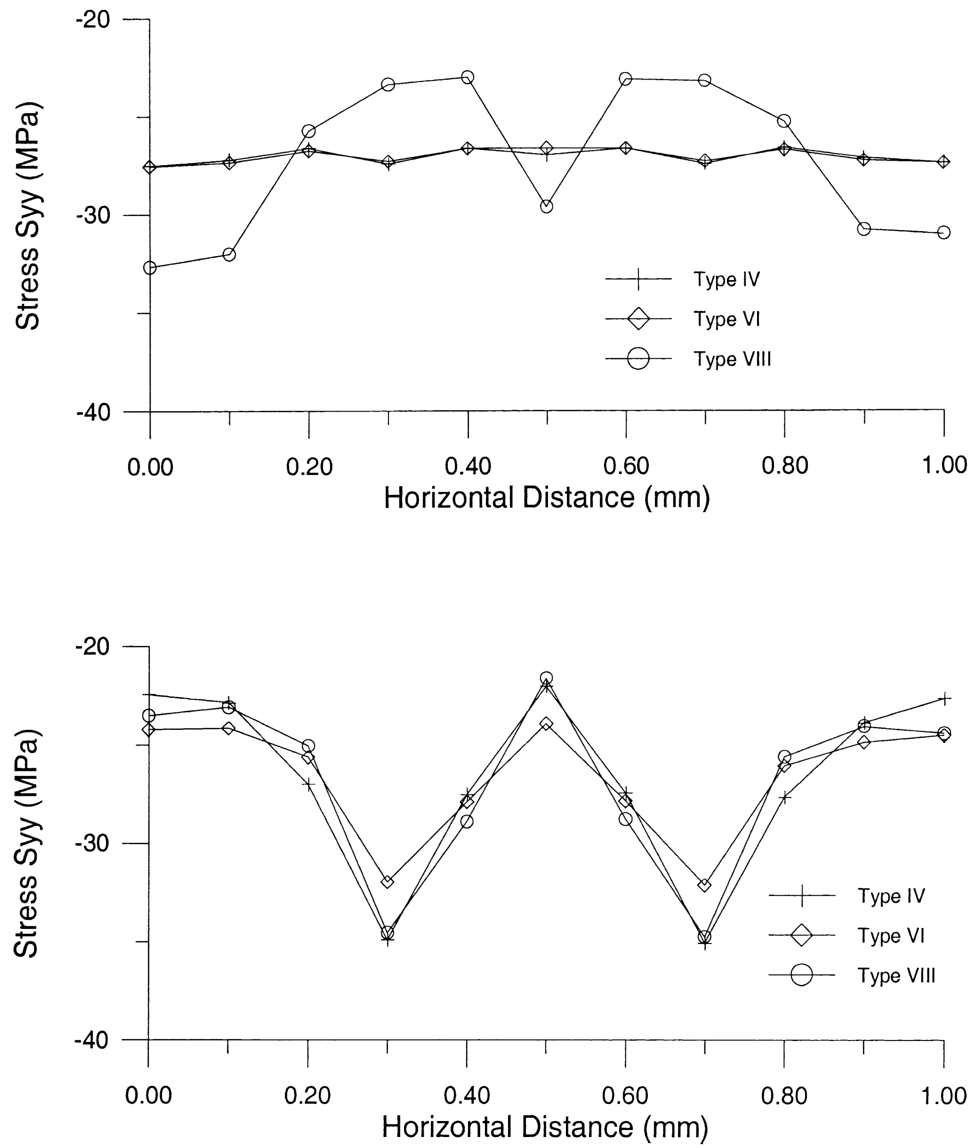


Fig. 6. (a) Stress Syy for section B–B for E_{iz} = 2000 N/mm^2. (b) Stress Syy for section B–B for E_{iz} = 6000 N/mm^2.

Note that all regions of the models develop similar values for the vertical displacement Uy. The maximum values for Uy are achieved when the modulus of elasticity of the ITZ is set at its minimum value (E_{iz}/E_{cp} = 0.25) and for the models which include four sand particles. These displacements are reduced as the modulus of elasticity of the ITZ increases. The maximum values of vertical displacement for the thinner ITZ bands are less than these for the thicker ITZ bands.

In Fig. 6a,b, comparative results of the vertical stresses (Syy) for model Types IV, VI, and VII are presented. The influence of distance between the aggregate particles can be observed for constant ITZ properties (models IV and VII). Decreasing this distance (model VII) leads to an increase in the vertical stresses developed at the cement paste region, especially when the modulus of elasticity of the ITZ is set at its minimum value (E_{iz}/E_{cp} = 0.25) as shown in Fig. 6a. For higher values of E_{iz}, vertical stresses remain constant for various model geometries (Fig. 6b). In addition, Fig. 7a,b presents the vertical stress (Syy) distribution, for different widths of the ITZ (models III and IV). It is shown that higher ITZ widths result in higher vertical stresses in the body for low E_{iz} values (Fig. 7a), while the width of the zone does not affect vertical stresses for higher E_{iz} values (E_{iz}/E_{cp} = 0.75) as shown in Fig. 7b.

In conclusion, the maximum tensile stresses tend to concentrate mainly in the ITZ that lays between the cement paste and the aggregates, when the elastic modulus and the width of the ITZ take their minimum values in the parametric analysis described above. These stresses could lead to the development of microcracks along these regions,

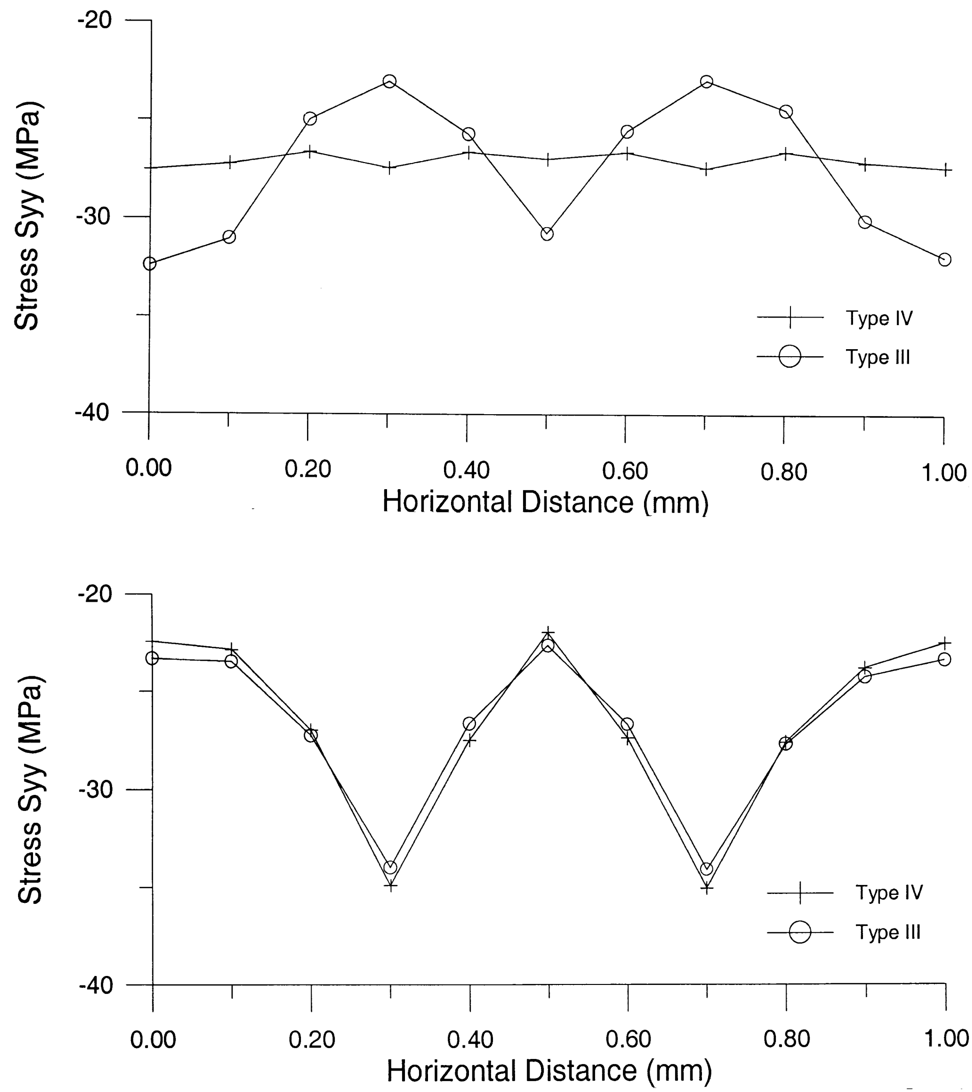


Fig. 7. (a) Stress Syy for section B–B for E = 2000 N/mm^2. (b) Stress Syy for section B–B for E = 6000 N/mm^2.

which in turn could lead to the failure of the concrete mixture. Laboratory work has indicated that in many cases concrete failure occurs around the aggregate particles [15]. These results are supported by the numerical analysis presented here. The lower the properties of the ITZ, the higher the stresses that concentrate in that region and may lead to or promote failure. It should also be noted that since concrete is a dynamic material whose mechanical properties are changing with time, this type of behavior may only be appropriate for a particular timeframe in the life of a concrete block.

Further work in this subject should include a further and in-depth examination of the properties of the ITZ. The parametric analysis should include a wider range of values especially in the lower region. As it is widely accepted that the ITZ demonstrates an elastoplastic behavior, a non-linear analysis should be performed. Finally, more variables could be added during the design of the models, such as a wider range of sizes and shapes for the aggregates and/or the interfacial zone in order to simulate the real conditions as closely as possible.

References

[1] E.J. Garboczi, D.P. Bentz, Digital simulation of the aggregate–cement paste interfacial zone in concrete, J Mater Res 6 (1) (1991) 1996–2001.

[2] R.T. Coverdale, H.M. Jennings, Computer modelling of microstructure of cement-based materials, in: A.K. Mullick (Ed.), Proceedings of the 9th International Congress on the Chemistry of Cement, National Council for Cement and Building Materials, New Delhi, India, 1992, pp. 16–21.

[3] K. van Breugel, Numerical simulation of hydration and structural development of cement-based materials, in: A.K. Mullick (Ed.), Proceedings of the 9th International Congress on the Chemistry of Cement, National Council for Cement and Building Materials, New Delhi, India, 1992, pp. 22–27.

[4] E.J. Garboczi, D.P. Bentz, Analytical formulas for interfacial transition zone properties, Adv Cem Based Mater 6 (1997) 99–108.

[5] C.M. Neubauer, H.M. Jennings, E.J. Garboczi, A three-phase model of the elastic and shrinkage properties of mortar, Adv Cem Based Mater, 4 (1996) 6–20.
[6] E.J. Garboczi, D.P. Bentz, The effect of the interfacial transition zone on concrete properties: The dilute limit, Proceedings of the Fourth Materials Conference, November 1996.
[7] E. Schlangen, E.J. Garboczi, Fracture simulations of concrete using lattice models: Computational aspects, Eng Fracture Mech 57 (2/3) (1997) 319–332.
[8] E.J. Garboczi, D.P. Bentz, Computer-based models of the microstructure and properties of cement-based materials, in: A.K. Mullick (Ed.), Proceedings of the 9th International Congress on the Chemistry of Cement, National Council for Cement and Building Materials, New Delhi, India, 1992, pp. 3–15.
[9] E.J. Garboczi, Stress, displacement and expansive cracking around a single spherical aggregate under different expansive conditions, Cem Concr Res 27 (4) (1997) 495–500.
[10] K. Mitsui, Z. Li, S.P. Shah, New quantitative method to characterize the interfacial properties between aggregate and cement paste, CANMET/ACI International Workshop on Advances in Concrete Technology, May 11–13, Athens, Greece, 1992.
[11] X.-H. Zhao, W.F. Chen, Stress analysis of a sand particle with interface in cement paste under uniaxial loading, Int J Numer Anal Methods Geomech 20 (1996) 275–285.
[12] G. Ramesh, E.D. Sotelino, W.F. Chen, Effect of transition zone on elastic moduli of concrete materials, Cem Concr Res 26 (4) (1996) 611–622.
[13] P.S. Theocaris, G.E. Stavroulakis, P.D. Panagiotopoulos, Calculation of effective transverse elastic moduli of fiber-reinforced composites by numerical homogenization, Compos Sci Technol 57 (5) (1997) 573–586.
[14] P. Simeonov, S. Ahmad, Effect of transition zone on the elastic behavior of cement-based composites, Cem Concr Res 25 (1) (1995) 165–176.
[15] E. Chatzopoulou, Numerical modeling of mechanical behavior of a cubic concrete specimen concentrating to the interfacial zone between cement paste and aggregate, Diploma Thesis, Dept. of Mineral Resources Engineering, Technical University of Crete, Greece (in Greek), 1997.
[16] M.D. Cohen, A. Goldman, W.-F. Chen, The role of silica fume in mortar: Transition zone versus bulk paste modification, Cem Concr Res 24 (1994) 95–98.