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A numerical method for predicting the elastic modulus of concrete made with two different aggregates*

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Abstract: Experimental and theoretical research showed that in predicting concrete's elastic modulus, it should be modelled as a three-phase composite material at a mesoscopic level, consisting of aggregates, interfacial transition zone (ITZ) and cement paste, and that the proportions, mechanical properties and interaction of the three phase constituents should all be considered in the prediction. The present paper attempts to develop a numerical method that can predict the elastic modulus of three-phase concrete made with two different aggregates. In this method, the mesostructure of concrete is simulated and the lattice type model is modified to take into account the mechanical properties of the cement paste, ITZ, and fine and coarse aggregates of concrete. The finite element method is then employed for analyzing the stress and strain in concrete and therefore for determining its elastic modulus. Finally, the developed numerical method is verified by comparison with the experimental results obtained from the research literature. The paper concludes that the numerical method can predict with reasonable accuracy the elastic modulus of concrete made with two different aggregates.

Key words: Concrete, Elastic modulus, Lattice type model, Finite element method
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INTRODUCTION

Elastic modulus of concrete is an important mechanical parameter for the design and assessment of reinforced concrete structures and as such has been studied extensively both experimentally and theoretically (Anson and Newman, 1966; Ramesh *et al*., 1996; Garboczi and Bentz, 1997; Li *et al*., 1999). Theoretical analysis has confirmed that, when the interfacial transition zone (ITZ) in concrete is ignored, the theoretical lower bound of Hashin and Shtrikman bounds for elastic modulus of concrete is higher than the measured elastic modulus of concrete (Simeonov and Ahmad, 1995; Lutz and Zimmerman, 2005). This implies that the concrete should be modelled as a three-phase composite material at a mesoscopic level, consisting of aggregates, ITZ and cement paste (Ramesh *et al*., 1996; Li *et al*., 1999; Nie and Basaran, 2005). Although there exist numerous analytical and numerical methods that can predict the elastic modulus of concrete as a three-phase composite material (Garboczi and Bentz, 1997; Li *et al*., 1999; Li *et al*., 2003), they are merely applicable to concrete made with single aggregate, i.e., all aggregates in concrete are of the same elastic modulus. It is also appreciated that, for concrete made with two different aggregates, an approximate method has been developed for evaluating its elastic modulus (Yang and Huang, 1996). But the ITZ in concrete is not taken into account in this method. It is in this regard that a numerical method is proposed in the paper to evaluate the elastic modulus of concrete made with two different aggregates as a three-phase composite material.

In the proposed method, the mesostructure of concrete is simulated and the lattice type model is modified to take into account the mechanical properties of each phase constituent material. The elastic

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modulus of concrete is then determined by finite element method. Finally, the numerical method is verified with the experimental results obtained from the research literature.

SIMULATION OF THE MESOSTRUCTURE OF CONCRETE

As stated in the previous section, concrete made with two different aggregates, i.e., the elastic modulus of fine aggregate being different from that of coarse aggregate is considered in this paper. In order to predict the elastic modulus of the concrete as accurately as possible, detailed knowledge of the mesostructure of concrete is essential (Berryman, 2005). This can be achieved through simulating the distribution of aggregates and ITZs in concrete, since the mesostructure of concrete in practical use is random by nature. Through random simulation, the heterogeneity of concrete can be represented as realistically as possible. At present, due to the limitation on computer capacity and speed, the lattice type model is prevented from being applied to the three-dimensional stress analysis in the three-phase concrete. For this reason, the simulation of the mesostructure of three-phase concrete is limited to two dimensions in the paper.

In simulating the distribution of aggregates, it is reasonable to assume that aggregates of concrete, such as gravel, are spherical (Zheng and Li, 2003). The assumption of spherical aggregate is convenient for the generation of aggregates, the simulation of ITZ structure and the incorporation of the lattice type model. Although it is appreciated that the aggregate shape affects the elastic modulus of concrete somehow (Feng and Yu, 2001), the difference in elastic modulus induced by this assumption is negligibly small for normal concrete. Thus, at a given section of a concrete unit, the intersected aggregates are circular. Based on the theory of stereology (Li *et al*., 2003), the size distribution of the circular aggregates can be expressed as the cumulative distribution function in terms of the number of aggregates. The smallest aggregate diameter is taken as 1 mm, whereas the largest aggregate diameter varies from 4 to 32 mm for most practical applications. The simulation domain considered in the paper is a rectangle with sides of a and b. With the cumulative distribution functions for fine and coarse aggregates and rectangular simulation domain, the circular aggregates to be distributed in the simulation domain can be generated for a given fine aggregate area fraction A_{fa} and coarse aggregate area fraction A_{ca} (Li *et al*., 2003). Before placing the generated circular aggregates with various sizes into the simulation domain, they are arranged in descending order with respect to their sizes so that these aggregates can be more easily packed into the simulation domain. In order to produce the mesostructure of concrete that resembles real concrete in the statistical sense, the random sampling principle of Monte Carlo's simulation method is used for the distribution of aggregates. The random sampling is conducted by placing the generated aggregates one by one into the simulation domain in such a way that there is no overlapping with aggregates already placed. It has been shown that in actual concrete, although the ITZ thickness depends on factors such as water/cement ratio, it seems to be independent of the size of aggregates (Li *et al*., 1999). Thus, once all generated aggregates have been placed into the simulation domain, the ITZ structure can be reproduced by adding an ITZ layer of thickness h around each aggregate.

Based on this procedure, the mesostructure of concrete can be simulated for different aggregate area fractions, as typically shown in Fig.1 for a=100 mm, b=200 mm, and the Fuller aggregate gradation (Zheng and Li, 2003), where dark circles denote coarse aggregates and gray circles denote fine aggregates.

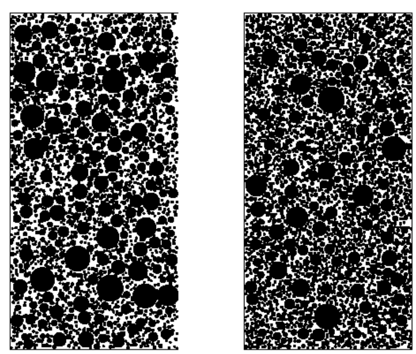
(a) (b)

Fig.1 Mesostructure of concrete for (a) A_{fa}=0.2 and A_{ca}=0.3; (b) A_{fa}=0.3 and A_{ca}=0.2

ELASTIC MODULUS OF CONCRETE

In finite element analysis, a mesh must be established first (Leite *et al*., 2004). At present, there are basically two types of mesh at a mesostructural level: the random lattice mesh and the regular lattice mesh (van Mier and van Vliet, 2003). The disadvantage of a random lattice mesh is that a large number of elements are needed to describe the mesostructure of concrete accurately since the elements are in a random order (Schlangen and van Mier, 1992). For this reason, an equilateral triangular lattice mesh with beam elements is chosen in the paper. Since the length of the beam elements strongly depends on the smallest aggregate diameter, a few elements are needed within the smallest aggregate to actually represent the mesostructure of concrete. Therefore, the side of beam elements, l_b, is set to be less than half the smallest aggregate diameter in the paper. The height of beam elements, h_b, is then equal to $0.68l_b$ (Schlangen and van Mier, 1992). A typical triangle lattice mesh with beam elements is shown in Fig.2. The total number of beam elements is generally in the range of 10^5 and 10^6. In finite element analysis of heterogeneous materials, formulation of element stiffness matrices is a key step to reach an accurate solution. As shown in Fig.2, there exist three interrelationships between a beam element and the aggregates: (1) the beam element is within a certain aggregate; (2) the beam element is within cement paste and; (3) the beam element intersects one or more aggregates. When the beam element is within a certain aggregate or cement paste, it is composed of homogeneous material and its element stiffness matrix can be obtained directly. When the beam element intersects one or more aggregates, it is composed of heterogeneous material. In this case, the beam element is divided into *n* sub-elements by the aggregates, cement paste and ITZs to remain homogeneous for each sub-element as shown in Fig.3. Its element stiffness matrix can be formulated by transfer matrix method (Li *et al*., 2003; Ellakany *et al*., 2004). With these element stiffness matrices, the stress and strain in the concrete element under any external load can readily be analyzed using finite element methods. For the purpose of determining the elastic modulus of concrete, only a uniform tensile or compressive strain ε_0 in the vertical direction applied at two edges of the concrete element is considered. The average stress σ_0 can be obtained based on the above finite element analysis. With both stress and strain, the elastic modulus of concrete, E_c, can be determined as follows:

$$E_c=\sigma_0/\varepsilon_0. \quad (1)$$

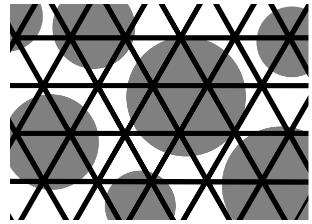

Fig.2 Triangular lattice mesh with beam elements

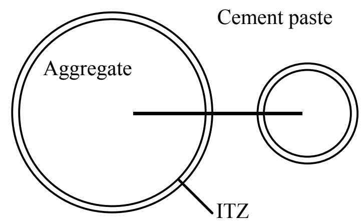

Fig.3 Intersection of a beam element

VERIFICATION OF THE NUMERICAL METHOD

To verify the developed numerical method, the experimental results on elastic modulus of concrete obtained by Anson and Newman (1966) are used for comparison. In their experiment, the water/cement is 0.5, the elastic moduli of cement paste, fine aggregate and coarse aggregate are respectively 12, 80 and 69 GPa, and the Poisson's ratios of cement paste and aggregate are respectively 0.25 and 0.15. The measured elastic modulus of concrete is shown in Table 1 for different fine and coarse aggregate area fractions.

Table 1 Comparison of numerical results with experimental results

A_{fa}	A_{ca}	E_c (GPa)		Relative error (%)
		Experimental	Numerical	
0.446	0.18	34.90	31.56	9.6
0.408	0.25	34.20	33.57	3.9
0.392	0.28	35.40	34.76	4.4
0.381	0.30	36.20	35.08	4.9
0.353	0.35	38.60	36.71	6.2

To compare with the experimental results, more information on the basic variables is necessary. This includes the Poisson's ratio, elastic modulus and thickness of ITZ. For ITZ it is extremely difficult to determine its elastic properties. Hashin and Monteiro (2002) presented an inverse method to evaluate the elastic properties of ITZ. According to their study, the Poisson's ratio of ITZ varies between 0.31 and 0.40.

In the paper, an average value of 0.35 is assumed for the ITZ. In evaluating the elastic modulus of ITZ, Lutz *et al*.(1997) assumed that, outside of each aggregate, the bulk modulus of ITZ varies smoothly as a power law function of radial distance from the center of the aggregate. An analytical expression was then formulated for the bulk modulus of concrete and compared with experimental data. From this comparison, it was inferred that the average elastic modulus ratio of ITZ to cement paste is 0.60. So in the verification, the elastic modulus of ITZ is taken as 7.2 GPa. Finally the ITZ thickness h needs to be known. According to (Zheng *et al*., 2005), h varies from 9 to 51 μm for normal concrete. So in the verification, h is taken as the average of the two bounds, i.e., h=30 μm.

With these variables known, the elastic modulus of concrete can be evaluated by the developed numerical method. The results are shown in Table 1, showing that the numerical results are in good agreement with the experimental results with an average relative error of 5.4%. Therefore, it is vindicated that the numerical method presented in the paper can predict with reasonable accuracy the elastic modulus of concrete made with two different aggregates.

CONCLUSION

A numerical method for predicting the elastic modulus of concrete made with two different aggregates is proposed in this paper, based on the simulation of the mesostructure of concrete and the finite element analysis of stress and strain in concrete. To represent the three-phase nature of concrete as realistically as possible in finite element analysis, the lattice type model has been modified to include the elastic modulus and thickness of ITZ. By comparison with the experimental results, the validity of the proposed numerical method has been verified. It can be concluded that the proposed numerical method can predict with reasonable accuracy the elastic modulus of concrete made with two different aggregates.

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