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Numerical and statistical analysis of elastic modulus of concrete as a three-phase heterogeneous composite

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ABSTRACT

This paper investigates the elastic modulus of concrete as a three-phase heterogeneous composite. Theoretically, the influence of aggregate and interfacial transition zone (ITZ) can be well characterized by the Ramesh model. Through generation of random aggregate structure, numerical samples of concrete are established and analyzed to calculate elastic modulus. It is shown that soft ITZ can greatly cancel the enhancement of aggregate while stiff ITZ cannot help much to strengthen concrete. The size of representative volume element of concrete is suggested in terms of expected error employing numerical–statistical approach. The required sample size with certain realization number is also calculated.

1. Introduction

Concrete material is thought to be a three-phase heterogeneous composite, with coarse aggregate randomly filled into mortar matrix in centimeter scale. In millimeter or smaller scale mortar matrix can be also considered as a heterogeneous material with fine aggregate randomly distributed in cement paste matrix. The interface between matrix and aggregate (fine or coarse), created by the presence of aggregate and known as interfacial transition zone (ITZ) [1], plays a significantly important role in both mechanical and transport properties of composite material [2–5]. Elastic modulus denoting the stiffness of material is regarded as one most important characteristic of concrete material in addition to strength. As a main component with high volume ratio, aggregate obviously has great influence on elastic modulus. In another aspect, ITZ also has remarkable impact on elastic modulus though it is only very thin soft shell surrounding aggregate with small volume ratio. Numerous efforts have been made to estimate the elastic modulus of concrete with much emphasis on aggregate and particularly ITZ [3,6,7].

Through theoretical, numerical and experimental approaches, the elastic modulus of concrete material has been extensively studied. Theoretically, the elastic modulus can be estimated by classic bound theory and effective medium theory, in which the aggregate is idealized as circular or spherical inclusion [3,8]. Some estimate schemes, which can take the influence of interfacial transition zone into account, consider the ITZ as concentric soft shell around aggregate and can give reasonably good estimate [6,9]. Considering the effect of inner geometry of concrete material and the influence of ITZ, numerical method has great adaptation to complex microstructure but faces great difficulty in handling the multi-scale features. For three-phase concrete material, the thickness of ITZ was reported as about several tenth micrometer [10]. It is far more smaller than the size of coarse aggregate, not mentioning the size of representative volume element (RVE), based on which numerical simulation can be carried out. Because of the multiscale characteristic of concrete material, efficient numerical simulation technique like finite element method will encounter great trouble to obtain proper mesh and solution [7,11]. Experiments were also widely carried out to study the influence of aggregate [12–14] while the effect of ITZ is incorporated into as well.

In solving elastic modulus of heterogeneous concrete material using both numerical simulation and experimental testing, the concept of representative volume element is generally introduced or implied. In literature there are various definitions of RVE, which are given from different viewpoints [15,16]. Accordingly, the determined RVE size would be different from one to another, such as elastic modulus, heat conductivity and fracture energy for quasi-brittle materials [15]. The existence of RVE is even problematic for concrete material in softening phase [16]. A classical RVE definition, reported by Hill from the view of elastic modulus, is introduced as a sample that is entirely representative of the whole mixture on average and contains a sufficient number of inclusions.

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And the overall modulus is macroscopically uniform and independent of applied boundary condition [17]. The actual representation of numerical or practical sample is essential to ensure the accurate numerical simulation or experimental measurement performed on them. The RVE size will be determined by numerical and statistical analysis in the sense of elastic modulus for concrete material [18].

The objective of this work is to investigate the influence of aggregate and ITZ on overall elastic modulus of concrete as well as its statistical properties. In Section 2, the realization of mesoscopic concrete structure and numerical solution of apparent elastic modulus are briefly introduced. Taking the influence of coarse aggregate and interfacial transition zone into account, the elastic modulus of concrete material is solved numerically and compared to the theoretical estimate from effective medium theories in Section 3. In Section 4 the statistical properties of elastic modulus of many random numerical realizations are investigated and the size of representative volume element is determined in the sense of elastic modulus. Finally, some conclusions are drawn out in Section 5.

2. Numerical model and analysis algorithm

2.1. Numerical model of three-phase concrete

To facilitate the numerical simulation and statistical analysis of elastic modulus, numerical sample of three-phase concrete material is firstly established. Herein the take-and-place method is adopted to generate two-dimensional inner geometry of concrete [19]. The aggregate is represented by angular polygon. The particle size is defined as the minimum width of circumscribed rectangular, the aspect ratio of which is defined as its elongation γ_{agg}. These definitions of particle size and aspect ratio are in well accordance with sieving test. According to the adopted particle size distribution and volume ratio, aggregate particles are taken and then randomly placed into a square matrix from large to small to realize the random aggregate structure (RAS) of concrete by a carefully designed Monte-Carlo algorithm. In the simulation below, the Fuller parabola is employed to describe the particle size distribution of dense graded coarse aggregate particles,

$$y = \left(\frac{D - D_{\min}}{D_{\max} - D_{\min}}\right)^{0.5} \tag{1}$$

where y denotes the weight ratio passing a sieve with aperture diameter D, and $D_{\max,\min}$ are the largest and smallest particle sizes, respectively. The volume ratio of coarse aggregate f_{agg} is retained as $f_{\text{agg}} = 0.40$, and $D_{\max} = 20$ mm, $D_{\min} = 5$ mm. The elongation of particles γ_{agg} is treated as a random variable observing continuous uniform distribution, abbreviated as $\mathrm{U}(a, b)$ with minimum value a and maximum value b. Two typical random aggregate structures of 150 mm square samples with $\gamma_{\text{agg}} \sim \mathrm{U}(1,2)$ and $\mathrm{U}(2,3)$ are shown in Fig. 1.

The interfacial transition zone is considered as a soft shell surrounding aggregate. After the realization of random aggregate structure, a thin layer with certain thickness is isolated from the interface between aggregate and matrix and identified as ITZ, as shown in Fig. 1. In literature, there are many experimental observations on the thickness of ITZ. For various concrete materials observed by different methods, the thickness of ITZ is also different but mainly located in the range of 20–100 μm [10,20–22]. To simplify the numerical simulation performed herein, ITZ depth is treated as a constant 100 μm since the thickness of ITZ seems to be independent of inclusion size [10]. Since the elastic modulus of concrete sample will be solved by finite element method, all the three phases are discretized with 6-node triangular element employing the free mesh function of general finite element analysis package "ANSYS". A typical detailed meshing in the domain around an aggregate particle is shown in Fig. 1, from which the phase transition can be seen clearly. The triangular element type adopted here has great adaptation to complex geometry of three-phase concrete material and good mesh quality is ensured. The requirement on the shape of all elements is satisfied to ensure good accuracy of FEM analysis. Besides, the mesh size of all triangular elements for the interfacial transition zone is small enough to estimate the effect of ITZ. Moreover, the mesh density is well organized from the ITZ to the nearby aggregates and matrix, as shown in Fig. 1. For the typical numerical sample of 150 mm square, there are about 710,000 nodes, 350,000 elements after meshing operation, which takes much of the computing time due to the complex geometry and very fine mesh around ITZ.

2.2. Analysis algorithm of elastic modulus

The elastic modulus of heterogeneous concrete composite is solved by average-field theory, which is often used to determine the effective properties of heterogeneous material from microscopic scale [23,24]. By defining effective mechanical properties, average-field theory can give the relation between volume average strain and stress of microscopically heterogeneous materials. Considering a volume element V made of heterogeneous material with an external boundary ∂V, the volume average stress $\bar{\sigma}_{ij}$ and strain $\bar{\varepsilon}_{ij}$ can be given as

$$\bar{\sigma}_{ij} = \frac{1}{V}\int_V \sigma_{ij}(\boldsymbol{x})\mathrm{d}V, \quad \bar{\varepsilon}_{ij} = \frac{1}{V}\int_V \varepsilon_{ij}(\boldsymbol{x})\mathrm{d}V \tag{2}$$

where $\boldsymbol{x}$ is the position vector. The generalized Hooke's law for such a volume element gives

$$\bar{\sigma}_{ij} = C^{\text{App}}_{ijkl}\bar{\varepsilon}_{kl}, \quad \bar{\varepsilon}_{ij} = S^{\text{App}}_{ijkl}\bar{\sigma}_{kl} \tag{3}$$

where C^{App}_{ijkl} and S^{App}_{ijkl} denote apparent stiffness tensor and compliance tensor, respectively. After solving the average strain $\bar{\varepsilon}_{ij}$ and

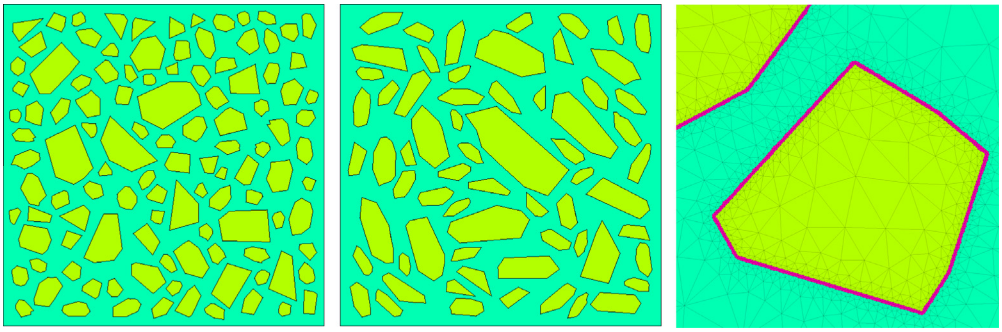

Fig. 1. Random aggregate structure with elongation $\gamma_{\text{agg}} \sim \mathrm{U}(1,2)$ (Left), $\gamma_{\text{agg}} \sim \mathrm{U}(2,3)$ (Middle) and a typical detailed part of generated mesh (Right).