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Effects of particle size distribution, shape and volume fraction of aggregates on the wall effect of concrete via random sequential packing of polydispersed ellipsoidal particles

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ABSTRACT

Concrete can be viewed as granular materials at the mesoscopic level. A specific distribution of aggregate particles in boundary layers, known as the wall effect, plays an important role in the mechanical properties and durability of concrete. However, the detailed and systematic experimental and simulated data about the wall effect of concrete is hardly adequate yet. Specially, the modeling study of spherical and two-dimensional (2D) elliptical aggregates distribution for the wall effect has been focused on in previous work, little is known about three-dimensional (3D) ellipsoidal aggregates. In the present work, based on a mesostructure model of concrete, the wall effect of concrete is quantified by configuration parameters such as the volume fraction, the specific surface area and the meaning free spacing of the solid phase. In addition, the influences of ellipsoidal particle size distribution (EPSD), shape and volume fraction (V_f) of ellipsoidal aggregates on the configuration parameters are evaluated by stereological methods and serial section analysis technique. Furthermore, the effect mechanisms of EPSD, shape and V_f are analyzed and discussed in this paper. The reliability of the statistical results is verified by experimental data and theoretical analytical results.

1. Introduction

At the mesoscopic scale, concrete can be considered as two-phase composite materials, composed of the random packing of irregular aggregate particles and the hydrated cement matrix into a formwork. Due to the effect of the formwork's walls, the configuration parameters of the mesostructure of concrete, such as the volume fraction V_V, the specific surface area S_V and the mean free spacing λ of the solid phase, in the neighborhood of the boundary layers is different from that at the center of the formwork. This phenomenon is known as the wall effect [1,2]. These configuration parameters play an important role in characterizing the influence of meso-/micro-structure of the interfacial transition zone (ITZ) (e.g., the thickness [3–5] and volume fraction [6–9] of ITZ, etc.) and physical properties (e.g., transport [10] and mechanical [11] properties, etc.) in concrete.

For instance, the volume fraction V_V of the solid phase is generally used to reflect the thickness of ITZ defined as the distance corresponding to the stable value of the curve of V_V from the boundary layers to the center of the mesostructure of concrete [3–5]. And the volume fraction of ITZ is strongly dependent on the thickness of ITZ and the specific surface area S_V of the solid phase [6–9]. Based on composite theory, many different kinds of multi-phase composite models have been developed to considered the influence of the meso-/micro-structure of ITZ on the effective physical properties (e.g., thermal/electrical conductivity, ion diffusivity, dielectric constant and elastic modulus, etc.) of concrete, such as

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the single/multi-layer composite sphere model [10,11], the generalized self-consistent model [12,13] and the differential effective medium model [14,15], etc. In these models, the most important parameter is the volume fraction of ITZ. Furthermore, during the drying process, the drying shrinkage strain energy of concrete is roughly correlated to the increment of interfacial energy induced by evaporation of water can be expressed as $\int_{r_p}^{r_\infty} \Delta\gamma S_V \,\mathrm{d}r$ [16,17], where S_V is the specific surface area of the solid phase and $\Delta\gamma$ is the increment of the surface tension caused by the transition between the solid–liquid interface to the solid–gas interface during the drying process. In other words, $\Delta\gamma = \gamma_{sg} - \gamma_{sl}$, where γ_{sg} and γ_{sl} are the surface tensions of the solid–gas interface and the solid–liquid interface [17], respectively. Considering no the damage evolution and the linear elastic deformation in concrete, the variation of interfacial energy can be regarded as the change of the strain energy during the drying process based on the principle of energy conservation. i.e., $\int_0^{\varepsilon} E\varepsilon d\varepsilon = \int_{r_p}^{r_\infty} \Delta\gamma S_V \,\mathrm{d}r$, where E and ε are the elastic modulus and the strain in concrete [17,18], respectively. On the other hand, the mean free spacing λ is the average of all unobstructed surface-to-surface distances to neighboring particles [19], of which the third power is usually conceived inversely proportional to global bond strength of concrete (i.e., $F = A/\lambda^{-3}$, where F and A and global bond strength and the Van der Waals constant). [4,20–22], as physical inter-particle bonding forces should have their share in building up "strength" particulate materials like concrete.

To investigate the gradients of these configuration parameters in the mesostructure of concrete, extensive research strategies have been implemented [3–5,23–25]. Early studies are mainly focused on the laboratory experiments and just produce a distribution on the volume fraction V_V of the solid phase [24,25]. For instance, Kreijger [24] and Yang et al. [25] introduced V_V firstly increased then got to a plateau from the boundary layers to the center of concrete by a series of sawed slice experiments and digital image analysis, and they concluded that the thickness of ITZ was equal to the minimum size of particles. However, the conventional experimental work is laborious and involves relatively large errors and uncertainties [26,27].

To overcome this difficulty, various random packing models of particles have been developed to access the gradients of these configuration parameters in the mesostructure of concrete [3–5,28–32]. For example, applying a spherical particle random sequential packing model, Zheng et al. [3,28] only displayed the gradient of V_V in concrete consisting of ascending, descending and horizontal parts, and they suggested that the thickness of ITZ was considered as the maximum diameter of spherical particles, which are inconsistent with the experimental results [24,25]. Subsequently, employing a discrete element model of spherical particles, Stroeven et al. [4,29–32] have introduced the gradients of the three configuration parameters (V_V, S_V and λ^{-3}) in the spherical particle packing model and revealed that the thickness of ITZ was of the order of a 1/3rd of the maximum grain size in the higher range of volume fraction ($0.61 - 0.44$) of aggregate particles [22]. Unfortunately, a major drawback in these studies is that all of the aggregate particles are assumed as spherical, which cannot represent the true shape of aggregate particles in concrete. Therefore, in the particle random packing models, it is necessary to consider a more suitable approximation for aggregate particles with realistic shape.

Recently, with the monodispersed and polydispersed 2D elliptical particle random packing models applied, Xu et al. [5,33,34] have presented the gradient of the area fraction of the solid phase and evaluated the dependences of the gradient on the shapes and sizes of ellipses, respectively. A similar work has also been investigated in a confined hard ellipse fluid [35]. However, these researches only stay in the 2D elliptical aggregate particles and little is known about the gradients of the three configuration parameters in the 3D non-spherical particle random packing model. Actually, as a more suitable approximation for the mesostructure of concrete, the random packing model of ellipsoidal particles has been extensively observed by various numerical algorithms, such as the random sequential algorithm [36,37], the discrete element algorithm [27,38–40], the molecular dynamic algorithm [41–43] and the mechanical contraction algorithm [44–46], etc. Consequently, in this work, the random packing model of polydispersed ellipsoidal particles representing the mesostructure of concrete, will be applied to access the gradients of the three configuration parameters (V_V, S_V and λ^{-3}).

In this paper, three steps will be considered. Firstly, a mesostructure model of the two-phase concrete will be constructed by means of the random packing of polydispersed ellipsoidal aggregate particles satisfied with a specific particle size distribution. Based on the mesostructure model, the dependence of the wall effect of concrete on various influencing factors such as particle size distribution, shape and volume fraction of particles will be presented in Section 3. Finally, the conclusion will be demonstrated in Section 4.

2. Mesostructure model of concrete

In the computer modeling technology, aggregate particles are usually modeled as spherical particles to study particle size distribution (PSD) in concrete [28–32]. However, EPSD has seldom been reported on until now. In this work, an equivalent diameter, which is defined as the diameter of a sphere having the same volume as that of an ellipsoid [36,37,47], is introduced to describe EPSD, as expressed in Eq. (1).

$$\begin{cases} D_{eq} = 2c\kappa^{-\frac{2}{3}} & \kappa \le 1 \\ D_{eq} = 2c\kappa^{\frac{1}{3}} & \kappa \ge 1 \end{cases} \tag{1}$$

where D_{eq} is the equivalent diameter of the ellipsoid, c and κ (i.e., if the ellipsoid shape is prolate, $\kappa = a/c$; if the ellipsoid shape is oblate, $\kappa = c/a$) are the semi-minor axis and aspect ratio of the ellipsoid, respectively. Thus, EPSD can be connected with PSD of spherical aggregates.