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Random non-convex particle model for the fraction of interfacial transition zones (ITZs) in fully-graded concrete

Wenxiang Xu [a,*], Zhongmei Han [a], Liang Tao [a], Qihan Ding [a], Huaifa Ma [b,*]

[a] Institute of Soft Matter Mechanics, College of Mechanics and Materials, Hohai University, Nanjing 211100, China

[b] State Key Laboratory of Simulation and Regulation of Water Cycle in River Basin, China Institute of Water Resources and Hydropower Research, Beijing 100048, China

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ABSTRACT

The structural configuration such as the fraction of interfacial transition zones (ITZs) has been found that can seriously impact the whole physico-mechanical properties of concrete. However, the fraction of ITZs is difficultly determined by traditional experimental methods and simple models proposed so far. In this work, a comprehensive numerical framework is devised to statistically obtain the fraction of ITZs around non-convex aggregates in fully-graded concrete. In the numerical framework, the authors generate a three-phase two-dimensional random non-convex particle model consisting of homogeneous cement paste, non-convex aggregates with a specific gradation and ITZs with a constant dimension, through a random sequential addition (RSA) scheme so as to characterize the geometric model of fully-graded concrete at a microscopic sale. The geometric morphology of a non-convex particle is mathematically parameterized in terms of the deformation of an ellipse-based cell. Such the operation can strictly govern the geometric shape of non-convex particle and precisely realize the topological geometry of an interfacial layer with a constant dimension to meet the requirement of the famous core-shell structure. Combining the proposed random non-convex particle model with the one-point probability function, we statistically analyze the fraction of ITZs by the Monte Carlo simulations. Plus, the influences of the geometric characteristics of aggregates including the shape, gradation, fraction and the maximum size and the ITZ dimension on the fraction of ITZs are systematically investigated in fully-graded concrete. Importantly, a quantitative manner on the effects of the geometric shape and gradation of non-convex aggregates is explored for the first time. As a critical ITZ property, the present contribution can be further drawn into assessing physico-mechanical properties of fully-graded concrete.

1. Introduction

It has been recognized that the interfacial transition zones (ITZs) are a weak phase along with aggregates and cement paste that develops mainly due to the so-called "wall effect" of cement particles packing against aggregate surface [1], which suggests that the generation of ITZs significantly depends on the geometrical surface information of aggregates. Also, microstructures of ITZs vary distinctively from what are found in bulk matrix, like greater porosity, precipitation of long portlandite crystals and greater ettringite content [2,3]. The physical features including the elastic modulus and the fraction of ITZs are of prominent importance in the prediction of effective physico-mechanical properties (macron homogeneous average responses) of concrete as a typical particulate composite, in terms of the micromechanics of composites [4–7]. Recent experimental researches have however examined the elastic modulus of ITZs using serial costly and time-consuming micron experiments like nanoindentation, scanning or back-scattered electron microscopy (SEM/BSE) [2,3]. The experimental results meet the limitations of accuracy and duplicability on sample preparations, especially for nanoindentation experiments [3]. Also, it is impossible to practically capture the fraction of ITZs through micron experiments, since ITZs are essentially a complex percolating network that neighboring ITZs possess an overlapping potential when the packing density of their surrounding aggregates added to in a certain value (0.4–0.5) in concrete [8].

Over the past two decades, previous efforts have been spent theoretically and numerically assessing the fraction of ITZs in concrete. In theoretical aspects, Garboczi and Bentz [9] proposed a theoretical formula to observe the fraction of ITZs around spherical aggregates in normal concrete (NC). Afterwards, such the formula was extended to the predictions of diffusivity and elastic modulus of NC as a three-phase composite containing spherical aggregates, ITZs and cement paste [10,11]. For sophisticated approximations on the geometrical morphologies of aggregates, some attempts to analytically research the fraction of ITZs around non-spherical aggregates have been tried, including three-dimensional (3D) ellipsoids [12], convex polyhedra [13] and spherocylinders [14]. Moreover, Xu and coworkers [15] recently developed a general theoretical framework for the fraction of ITZs around 3D arbitrary convex particles. Also, the effect of such the

* Corresponding authors.
E-mail addresses: xuwenxiang@hhu.edu.cn (W. Xu), mahf@iwhr.com (H. Ma).

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interfacial characteristic on the effective conductivity and elastic properties of concrete was further explored in the recent literature [8,12,16,17]. It should be borne in mind that the above theoretical efforts are based on the seminal work by Torquato and coworkers [18], whom developed a theory of the nearest-surface distribution functions to calculate the so-called spherical void "exclusion" probability. Nevertheless, the preceding 3D theoretical contributions are not suitable for the two-dimensional (2D) situation, since the scaled-particle theory [19] for the 3D case is entirely different from that for the 2D case in the derivation of the radial distribution function at the contact value [8,18]. Therefore, it raises concern on the fraction of ITZs around 2D non-spherical particles, specifically for the issue of non-convex particles. Alternatively, numerical simulations provide an optional means to observe the fraction of ITZs. It is a prerequisite to realize a close to realistic geometric model of concrete at a micron level. For instance, by establishing random particle models (RPM) that aggregates of various shapes are randomly dispersed in cement paste and a compliant (penetrable) layer with a constant dimension representing a ITZ are coated on the surface of each aggregate, which is known as the hard core-soft shell structure (HCSSS), several researchers [13,14,20,21] numerically evaluate the fractions of ITZs around aggregates with ellipsoidal, polyhedral and spherocylindrical shapes. Although these theoretical and numerical lines of research may provide guidance for understanding the fraction of ITZs, the assumption of convex aggregates is too idealistic to reflect morphological characteristics of real grains in concrete. Instead, they might have a combination of concave and convex shapes, namely, complex non-convex aggregates. To authors' knowledge, at present, there is still no related information on the fraction of ITZs around 2D complex non-convex aggregates in concrete. It is our intention in the present work to address this gap.

This study is the first to explore the fraction of ITZs around non-convex aggregates in fully-graded concrete. The authors attempt to present a numerical framework that couples 2D non-convex R PM for the microscopic geometric structure of fully-graded concrete with the random point sampling scheme the estimation the fraction of ITZs. Plus, the impacts of geometric features like the shape, gradation, fraction and the maximum size of non-convex aggregates on the fraction of ITZs are discussed in-depth. The rest of this article is organized as follows. Section 2 describes 2D non-convex RPM. Section 3 illustrates a numerical simulation strategy for the fraction of ITZs using the random point sampling scheme. In Section 4, some results are given and discussed. Finally, this article is completed with some concluding remarks in Section 5.

2. Non-convex random particle model (RPM) for fully-graded concrete

Normally, a mass fully-graded concrete (e.g., dam concrete) uses a two-graded, three-graded or four-graded mixture ratio, where the largest aggregate size is 80 mm or 150 mm and the coarse aggregate content is generally as high as 50 to 80%. In order to ensure the validity of numerical simulations, it is very crucial that the proposed RPM can truly reflect the aggregate gradation, content, geometry and spatial distribution. In this section, we describe a two-phase non-convex RPM that the gradation and content of aggregates satisfy the requirement of fully-gradation concrete. Herein, the geometric morphology of a non-convex particle is mathematically characterized through the deformation of an ellipse-based cell. A numerical strategy for the overlap detection between adjacent non-convex particles is subsequently presented. And then, a parametric equation for the topological geometry of an interfacial layer with a constant dimension is proposed to generate a three-phase non-convex RPM. It is worth mentioning that such the parametric equation for the ITZ geometry is more precise than the approximate realizations that reported by previous works [7,12–15,20,21].

2.1. Two-phase composite structure

2.1.1. Morphology of a non-convex particle

Considering the parametric equation of an ellipse-based cell is expressed by [22]

$$\mathbf{P}(u) = \begin{bmatrix} x(u) \\ y(u) \end{bmatrix} = \mathbf{R}\begin{bmatrix} a\cos(u) \\ b\sin(u) \end{bmatrix} \tag{1}$$

with

$$\mathbf{R} = \begin{bmatrix} \cos(\alpha) & \sin(\alpha) \\ -\sin(\alpha) & \cos(\alpha) \end{bmatrix} \tag{2}$$

where $\mathbf{P}(u)$ is defined as the 2D parameterized function of an ellipse-based cell. $\mathbf{R}$ is a rotational matrix; α is the rotation angle standing for the orientation of ellipse; a and b are its semi–major and semi–minor axes; u is a parameter in the range of 0 to 2π.

Some researchers [22–25] have put forward to generating a convex polygon through the deformations of a circle-based cell or an ellipse-based cell. In essence, a non-convex particle can also be generated by the geometric deformation of an ellipse-based cell. In the following, a contraction factor function is displayed to obtain a 2D non-convex particle geometry, which is defined by

$$B(w, \mathbf{a}_{0i}, \mathbf{r}_i) = B(\mathbf{x}) = \frac{\int_{w(\mathbf{x})}^{\infty} g(s)\mathrm{d}s}{\int_{-\infty}^{\infty} g(s)\mathrm{d}s} \tag{3}$$

with

$$w = w(\mathbf{x}) = (\mathbf{x} - \mathbf{a}_{0i})^2, \quad g(s) = \begin{cases} e^{\frac{1}{\left(s-r_1^2\right)\left(s-r_2^2\right)}} & 0 \le r_1^2 < r_2^2 \\ 0 & \text{others} \end{cases} \tag{4}$$

where $B(\mathbf{x})$ is the contraction factor (CF) applied to the contraction at a given domain of $[a_0 - r_2, a_0 + r_2]$. $\mathbf{a}_{0i}$ is the deformation center of ith subinterval defined below. $\mathbf{r}_1$ and $\mathbf{r}_2$ are the peak interval and regional boundaries, respectively, the relationship of which meets the requirement of $0 \le \mathbf{r}_1 < \mathbf{r}_2$. $w(\mathbf{x})$ denotes the distance from an arbitrary spatial position $\mathbf{x}$ to the deformation center. Considering the universality method of computation, the authors further use the Gauss integral to derive the CF [26]. It is worth stressing that the CF can be used as the shape descriptor of an arbitrary non-convex particle generated by Gauss integral of eight nodes.

The following strategy is demonstrated to construct the geometric morphology of a 2D non-convex particle.

(1) Suppose an arbitrary ellipse-based cell, the interval of its parameter u in the range of 0 to 2π is subdivided into n subintervals, and the parameter and center of each subinterval are denoted as $u_i = 2\pi i/n$ and $\mathbf{a}_{0i}$, respectively, where $i = 1, 2, \ldots, n$.

(2) In ith subinterval, randomly generate two axial CFs of β_{1i} and β_{2i} in the range of $[-0.16, -0.1]$. The selection of such the range originated from a series of trials is to ensure the generated non-convex particles close to the realistic geometric morphologies of aggregates. Additionally, the two CFs are specified as the form of diagonal matrix:

$$\mathbf{D}_i = \mathit{diag}(\beta_{1i}, \beta_{2i}) \tag{5}$$

In order to ensure the existence of the unique contraction point in individual subinterval, it is prescribed the center of the subinterval $\mathbf{a}_{0i}$ as the deformation peak to inward contraction. Also, $\mathbf{r}_1$ and $\mathbf{r}_2$ are usually predefined as 0 and the random point in the subinterval, respectively.