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A combined-alpha-shape-implicit-surface approach to generate 3D random concrete mesostructures via digital image processing, spectral representation, and point cloud

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HIGHLIGHTS

- An approach to decompose and simulate 2D aggregate shape profiles is suggested.
- Morphological and spectral characteristics of aggregates are examined.
- A procedure to represent and simulate 2D microcracks in concrete is developed.
- A method to construct 3D aggregate point clouds is presented.
- An algorithm to generate 3D aggregate microstructures is proposed.

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ABSTRACT

Concrete aggregates have a random and complex shape, which has been shown to affect the mechanical properties of concrete. Commonly, they are approximated as spheres or polyhedra in 3D cases, or further simplified as circles or polygons in 2D cases. This study presents a numerical procedure for the stochastic characterization and representation of the aggregates and microcracks in concrete and the generation of virtual 3D random concrete mesostructures. Central to the proposed simulation method is the generation of realistic 3D aggregate point clouds based on an improved decomposition scheme and the conversion of the point clouds to 3D aggregate microstructures using a hybrid alpha-shape-implicit-surface algorithm. To optimize the simulation results, an image processing procedure and a set of representative aggregates are developed. It is shown that the proposed procedure is capable of reproducing high-quality concrete mesostructures with microcracks, which opens the door to unravelling complex microstructural behaviors of cement-based materials.

1. Introduction

Concrete refers to a heterogeneous multi-phase composite mixture that is mostly comprised of filler materials including coarse aggregates such as natural gravels and fine aggregates such as sand as well as binder materials such as cement. When mixed with water and (where needed) performance-enhancing additives, the mixed product first turns into a fluid form that can be molded or cast as desired and then hardens into a solid and rigid material that can be used in a variety of engineering applications. As the most ubiquitous construction material in the world, concrete has found widespread applications in a plethora of engineered structures including buildings, bridges, dams, tunnels, nuclear power plants, just to name a few.

Although it is anticipated that concrete will continue to be in high demand in the future, the concrete and cement industry is facing unprecedented challenges [1–3]. One of the grand challenges in the concrete science is that concrete possesses an exceedingly complex multiscale internal structure. In particular, as exhibited in Fig. 1, concrete materials are heterogeneous on the mesoscale, the mesostructure of which is comprised of aggregates and mortar as well as the Interfacial Transition Zone (ITZ) between them. The mechanical behavior of concrete at the macroscopic level is strongly dependent on the characteristics of the individual constituents at the finer mesoscopic level. For instance, it has been shown that the shape and surface texture of coarse aggregates can exert considerable impact on the properties of concrete (e.g.,

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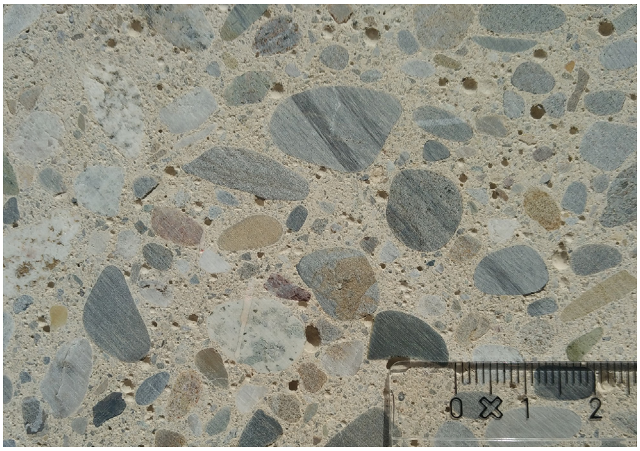

Fig. 1. Illustration of concrete mesostructure with aggregates made of natural gravels.

among others, [4–14]). In particular, the workability of concrete is largely influenced by the roundedness and angularity of the aggregates because aggregates with rougher surface textures tend to have more voids than those with smoother surface textures. As a consequence, more water is needed in the production of workable concrete [4–7]. In addition, the strength and fracture properties of concrete are closely related to the shape and surface texture of the aggregates in concrete [8–13]. For one thing, the interfacial bond between the aggregate and the cement paste as well as the mechanical bond strength is dependent on the surface roughness of the aggregates [12]. For another, the stresses upon which the cracks in the cement paste and aggregates initiate and propagate are associated with the shape of the aggregates [13]. Furthermore, the shape of aggregates can alter the microstructure of mortars, thus affecting the transport properties of mortars and, in turn, the chloride diffusivity in concrete [14].To gain insight into these aforementioned intricate micro-mechanisms, an accurate description of the microstructure of aggregates in concrete is warranted.

Nonetheless, while the rapidly increasing computing power has made possible simulating the complex microstructure of concrete and probing into its microstructural behavior, currently, there are still a number of outstanding issues that are present in the characterization and representation of concrete aggregates due to their random and complex grain structures. For these reasons, a number of research works have been devoted to the morphological description and simulation of concrete aggregates. For instance, one of the commonly utilized approaches for the representation of concrete aggregates is to approximate them using basic geometric shapes such as circles, ellipses, and polygons in the Two-Dimensional (2D) case. Along this line, Xu and his co-workers [15] approximated 2D aggregate shapes by way of ellipses. Taking a different approach, Wang et al. [17] modeled the 2D shape of concrete aggregates using harmonic functions to characterize the shape of natural gravels and polygons to approximate the shape of crushed rocks. Similarly, Du and Sun [18] also developed an algorithm for the generation of 2D arbitrary polygonal aggregates. On the other hand, Kim and Abu Al-Rub [19] compared the differences in the mesoscale modeling of concrete RVE samples considering different aggregate shape approximations including circles, hexagons, pentagons, tetragons, and arbitrary polygons. However, although the aforementioned simplified representation approaches allow for approximately accounting for the shape effects of aggregates, it is not capable of capturing the multifaceted details of real aggregate microstructures and thus elucidating the many complex micromechanics-based phenomena. In order to better describe the complex shape of random particle objects, Mollon and Zhao [21] developed a numerical approach for the simulation of realistic sand particles based on the Fourier Descriptor Method (FDM) [24–28]. It is however noted that their approach is intended for sand particles, which is not readily applicable to concrete aggregates due to the different particle shape and size characteristics of concrete coarse aggregates. Despite the tremendous potential and promise of the FDM, there are a couple of problems that are involved in the modeling of concrete aggregates using the FDM. First, as pointed out by Wang et al. [17], natural gravel aggregates can be simulated by representing their boundary contours through the summation of harmonic functions in polar coordinates, whereas concrete aggregates produced by crushing should be modeled differently because of their angular particle shapes. Thus, the FDM seems more suited to the modeling of natural gravel type aggregates due to the utilization of Fourier series in the simulation process. For crushed rocks that possess sharp-edged and angular characteristics, the FDM may not be able to simulate the flakiness and elongation of crushed rock aggregates. Second, although the FDM provides a most valuable tool for the realistic generation of arbitrary shaped particles, they, generally, bear limited association with actual particles. However, since the morphological characteristics of concrete aggregates may vary considerably from site to site, to generate aggregate shape profiles that are compatible with prescribed aggregate samples, the more sophisticated conditional simulation schemes that can incorporate the local information of concrete aggregates are necessary. In this way, the generated aggregate shape profiles not only exhibit realistic morphological features, but also inherit the physical characteristics of the predefined aggregate samples.

Indeed, 2D aggregate computational models have provided us a pragmatic approach to investigate the physical mechanisms underlying the many phenomena of the concrete material that are hard to be experimentally explored. However, these 2D models only serve as a qualitative way to understand a real Three-Dimensional (3D) problem. In case that a more thorough comprehension to the problem is sought, 3D aggregate models should be utilized instead. In this context, Kim and Abu Al-Rub [19], Wriggers and Moftah [20], Sobolev and Amirjanov [33] adopted spheres to simulate concrete aggregate particles and examined the mesoscopic damage behaviors of concrete RVE samples. On the other hand, Xu and his co-workers [16] emulated aggregate particles via ellipsoids. To better quantify the shape of real 3D sand particles, Mollon and Zhao [22,23] developed numerical methods for the generation of virtual 3D particles using Random Field Theory (RFT) and the Fourier Descriptor Method (FDM) [24–28]. In a different way, Garboczi, Grigoriu, and their co-workers [29–31] put forward spherical-harmonic-based schemes for the mathematical characterization and representation of 3D concrete aggregate particles. It should be noted that while the modeling of 2D aggregate shape profiles has been receiving relatively considerable research attention, fairly limited research efforts have been directed toward the development of 3D aggregate models due to the complexities involved. On a further note, in view of the current image scanning and processing techniques such as 3D scanning and printing, fast and reliable computational algorithms that can fully exploit these advanced imaging techniques and generate realistic 3D aggregate microstructures are still lacking.

Particularly, 3D printing offers tremendous possibilities for fabricating more innovated, customized, and environmental friendly concrete aggregates. More specifically, the benefits of exploiting the 3D printing technique for concrete aggregates include: (i) 3D printing supports the creative transformation of computer generated 3D aggregate models into physical objects to be used in experimental research. With 3D printing, it is possible to precisely control the size, shape, and surface texture of concrete aggregates,