AGGREGATE SHAPE EFFECTS ON THE MECHANICAL PROPERTY OF CONCRETE UNDER TENSILE LOADING: (1) SIMULATION OF ONE PARTICLE SYSTEM

Lin Liu (1), Huisu Chen (2), Zhigang Zhu (2), Zhiwei Qian(3)

(1) College of Civil and Transportation Engineering, Hohai University, Nanjing 210098, China
(2) Jiangsu Key Laboratory of Construction Materials, School of Materials Science and Engineering, Southeast University, Nanjing 211189, China
(3) Faculty of Civil Engineering and Geosciences, Delft University of Technology, 2628CN Delft, The Netherlands

Abstract

Investigations on the mechanical properties of concrete by computational modeling mostly were based on the meso-structure of concrete with spherical particles in the past decades. It may result in a significant discrepancy in simulations by ignoring the aggregate shape effects. In this study, the aggregate shape effects on the mechanical properties of concrete under tensile loading are explored by 3D numerical modeling. Preliminary simulations are carried out on one particle system. The meso-structures of one spherical aggregate, one ellipsoidal aggregate and one irregular shaped aggregate are constructed respectively. Then, the constructed meso-structures are digitalized into voxels, and 3D lattice fracturing analysis is performed on the digitalized meso-structures by applying tensile displacement. In this study, the load-displacement curve, load at first crack, tensile strength and crack propagation are presented and discussed.

1. INTRODUCTION

Mechanical properties of concrete are closely related to its corresponding micro-/meso-structures. Based on a particle packing model, by coupling with a specific algorithm, the mechanical properties of cement-based composite materials can be estimated [1-5]. The particle packing effects on the mechanical properties including Young’s modulus, tensile strength, toughness, fracture energy and so on have been studied by some researchers in 2D [1-4] and attempted by Azéma et al. in 3D [5].

In order to figure out aggregate shape effects on the mechanical property of concrete, enhanced understanding of the fracturing process of one particle system would be beneficial. In this study, the aggregate particle is modeled as a sphere, an ellipsoid with κ=3 (κ is the
aspect ratio), and an irregular shaped particle. The corresponding mechanical properties of concrete are predicted by employing a 3D lattice fracture model. The load-displacement curve, load at first crack, tensile strength and crack propagation are presented and discussed.

2. GENERATION OF MESOSTRUCTURES

The constructed particles (e.g. spherical, ellipsoidal with κ=3 and arbitrary-shaped) are illustrated in figure 1. Figure 1(b) and 1(c) show ellipsoidal particles whose semi-major axis is along x and y direction respectively. Based on a Fourier series (2D case) or a spherical harmonic series (3D case), the packing systems of arbitrary-shaped particles have been constructed in literature [6-9]. In this study, with the assistance of x-ray tomography and a spherical harmonic series, a star-shaped particle that is close to realistic arbitrary-shaped grains is constructed, see figure 1(d).

The constructed particles are located in the center of a box of 100mm length with a 0.05 particle volume fraction to simulate concrete mesostructures. The meso-structures are then digitalized into voxels, represented by aggregate or paste phase. The particle is assumed as aggregate. For mesostructures illustrated in figure 1, 100³ voxels are generated. Uniaxial tensile loading will be performed on the generated mesostructures in the following work.

![Mesostructures of one particle](image)

(a) Spherical  (b)Ellipsoidal (semi-major axis parallel to x direction)  (c) Ellipsoidal (semi-major axis parallel to y direction)  (d)Irregular shaped

Figure 1: Mesostructures of one particle

3. 3D LATTICE FRACTURE MODELING

3-D lattice fracture model can be utilized to analyze the fracturing process of a material in question introduced by external loading [10-12] or internal physical and chemical actions [13-15]. In this section, 3-D lattice fracture model is employed to simulate the uniaxial tensile loading test by which the load-displacement curve, cracks creation and propagation and tensile strength can be obtained.

Three stages are defined to make the modeling procedures clear: pre-processing, fracture processes simulation and post-processing. In the pre-processing stage, a lattice network is first constructed. Each lattice node is generated in the center of a solid voxel, and all these nodes
are connected by lattice elements. Theoretically, the lattice node can be located in a specific range of the voxel with a given randomness. The randomness is between 0 and 1. In order to systematically compare the fracturing behavior of mesostructures with different shaped aggregates, the randomness is set to 0. Therefore, the lattice node is generated in the center of the solid voxel. The local mechanical properties (Young’s modulus $E$, shear modulus $G$ and tensile strength $f_t$) assigned to every lattice element are determined as the clarification in table 1 [12]. Free boundary conditions in $y$ and $z$ directions are set when the tensile loading is applied in $x$ direction.

Table 1 Mechanical properties of lattice elements [12].

<table>
<thead>
<tr>
<th>Elements</th>
<th>Young’s modulus (GPa)</th>
<th>Shear Modulus (GPa)</th>
<th>Tensile strength (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aggregate</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Aggregate-aggregate</td>
<td>70</td>
<td>29</td>
<td>24</td>
</tr>
<tr>
<td>Paste</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Paste-paste</td>
<td>12.8</td>
<td>5.3</td>
<td>20</td>
</tr>
<tr>
<td>ITZ</td>
<td>Aggregate-paste</td>
<td>22</td>
<td>8.9</td>
</tr>
</tbody>
</table>

4. SIMULATION RESULTS AND DISCUSSION

By applying a prescribed displacement, the load applied on the sample can be obtained by the kernel solver in 3D lattice analysis. Figure 2 illustrates the load-displacement curve of virtual concrete of different shaped aggregate. It is found that at the same aggregate volume fraction, concrete of a spherical particle shows the largest capacity resisting to uniaxial tensile loading and deformation. The tensile strength of concrete with an ellipsoidal particle whose semi-major axis is vertical to the loading direction is second large. For the case of ellipsoidal particle whose semi-major axis is parallel to the loading direction, the concrete display the weakest capacity resisting to the mechanical loading. For the case of irregular shaped particle, the concrete exhibits a modest capacity on resisting to uniaxial tensile loading and deformation.

The first crack initiated during the loading process is given in figure 3. It is found that at the initiation of first crack, the displacement and load are smallest for ellipsoidal particle whose semi-major axis is parallel to the loading direction. While the last cracking sample (i.e., first crack occurs) is the ellipsoidal particle whose capacity resisting to loading is weakest. For the case of spherical particles, it displays a modest loading at cracking. This is slightly different from the trends shown in figure 2. This is related to the propagation of cracks in concrete. For the case of irregular shaped particle, again, the concrete exhibits a modest behavior on first crack initiation.

Propagation of cracks in concrete during the loading process is given in figure 4 to figure 7. All samples exhibit the same phenomenon. One element of ITZ phase parallel to the loading direction first breaks. That is the creation of first crack. Then, propagation of cracks
around the first crack happens and all the broken elements are of ITZ phase. Later, another element of ITZ phase parallel to the loading direction breaks and propagation of cracks around it happens with ITZ elements fracturing. At somewhere, the element of paste phase parallel to the loading direction breaks and propagation of cracks around it also happens but with paste elements fracturing. Transverse crack is formed and the whole structure is broken along the transverse crack.

Figure 2: Load-displacement curve of virtual concrete of different shaped aggregate.

Figure 3: Load-displacement curve around the first crack initiation.
Figure 4: Propagation of cracks in concrete of spherical particle.

Figure 5: Propagation of cracks in concrete of ellipsoidal particle whose semi-major axis is parallel to the loading direction.

Figure 6: Propagation of cracks in concrete of ellipsoidal particle whose semi-major axis is vertical to the loading direction.

Figure 7: Propagation of cracks in concrete of arbitrary-shaped aggregate.
5. CONCLUSION

Enhanced understanding of the fracturing process of one particle system is of significance to explore aggregate shape effects on the mechanical property of concrete. In this study, concrete of one aggregate particle of spherical, ellipsoidal and irregular shapes is generated, and its corresponding mechanical properties are investigated by 3D lattice fracture model. The load-displacement curve shows that concrete of spherical particle has the biggest capacity resisting to the uniaxial tensile loading, and the second large is for the case of ellipsoidal particle whose semi-major axis is vertical to the loading direction. For the case of ellipsoidal particle whose semi-major axis is parallel to the loading direction, the concrete displays the weakest capacity resisting to loading as well as crack initiation. For the case of irregular shaped particle, the concrete exhibits a modest behavior. From the propagation of cracks during loading, it is observed that the elements of ITZ phase parallel to the loading direction first break. Once one element of paste phase parallel to the loading direction breaks, propagation of cracks around it happens and transverse crack is formed. The whole structure is broken along the transverse crack.

This study exhibits concrete fracturing of one spherical, ellipsoidal and irregular shaped particle, further studies on other shaped particles and multi-sized particle packing systems will be explored in future research.

ACKNOWLEDGEMENT

The financial supports of National Natural Science Foundation of China via Grant No.51308187, and Natural Science Foundation of Jiangsu Province via Grant No. BK20130837, are greatly acknowledged. The China Postdoctoral Science Foundation (No. 2013M531266), Jiangsu Postdoctoral Science Foundation (No.1202022C), the foundation from State Key Laboratory of High Performance Civil Engineering Materials (No. 2012CEM005) and Jiangsu Key Laboratory of Construction Materials in Southeast University (No.2012CEM01) are also greatly acknowledged.

REFERENCES