Three-dimensional Micromechanical Modeling of the Particulate Material using X-ray Computed Tomography (CT) Images

(X-ray 단층 촬영 이미지를 이용한 입상재료의 3차원 모델링)

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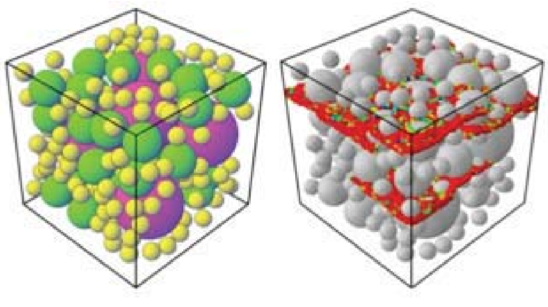
All construction materials, strictly speaking, such as steel, concrete, asphalt concrete, fiber reinforced polymer (FRP), and timber are not homogeneous materials but heterogeneous composite materials. Especially, concrete can be considered as a three-phase composite material consisting of mortar matrix, aggregate, and interfacial transition zone (ITZ), and asphalt concrete also has three components-aggregate, mastic, and void-at the microscopic scale. However, the majority of the analytical research on the inelastic and damage behavior of cementitious materials including asphalt concrete has been focused on treating them as a homogeneous material at the macroscopic scale which did not allow one to establish the microstructure-property relationship for designing better and superior fracture-resistant cementitious materials. This is mainly because the properties and role of each component, especially the properties of the ITZ, are not easy to be measured experimentally, because the realistic 3-D modeling is extremely difficult, and because the computational cost was very high in the past.

However, the recent advances in understanding the characteristics of the ITZ and other components and the developments in computational power made it possible to simulate effectively the micro-mechanical behavior of cementitious materials. On the other hand, the realistic three dimensional modeling of the material considering actual aggregate (or particle) shape, distribution, and gradation is still a challenging task because it is not simple to obtain inside information of material. With these reasons, almost all, but not much, 3-D mesoscopic level analysis of cementitious material, as shown in Figure 1, is based on two main assumptions that: (1) several sets of different sized spherical or ellipsoidal shape aggregates are randomly distributed; and (2) fine aggregates less than certain size are generally excluded in the model for the simplicity of modeling.



(a) (b)

Figure 1. 3-D spherical shape aggregate model for concrete: (a) analysis model and (b) tensile damage distribution

Using the 3-D spherical shape aggregate model which is also one of the most advanced analysis model for particulate material and most widely used, a variety of micromechanical behavior, such as aggregate size, distribution, and volume fraction effect, damage localization due to moisture and heat flow, and anisotropic crack propagation can be effectively simulated at the meso-scale level. In spite of these strong advantages, the regular shape aggregate model has still some drawbacks that the aggregate shape effect cannot be investigated and the stress concentration at the sharp tip of the aggregate which determines the initiation of damage is neglected.

In order for the more realistic micromechanical simulations of particulate material under various loading conditions, 3-D micromechanical simulations with actual shape, distribution, gradation, and volume fraction of particles are highly desirable. However, there have been very limited attempts to model the 3-D microstructure of concrete considering actual inside configurations due to the high complexity and very expensive computational cost. Mathematical approach, such as Fourier series analysis, spherical harmonic series, and wavelet analysis is one of the representative attempts to quantify the form, angularity, and texture of granular material, and one example of 3-D aggregates generated using spherical harmonic series are shown in Figure 2.

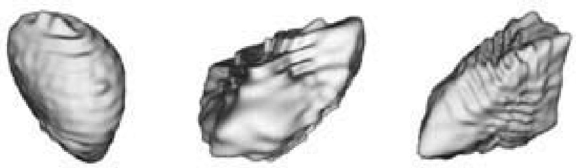


Figure 2. 3-dimensional profiles of aggregates

Although the mathematical methods are effective and efficient way to quantify the characteristics of each aggregate and can also be used to construct 3-D microstructure simulation model with distributing aggregates statistically, it is highly complicate and laborious.

From a decade ago, X-ray computed tomography (CT) images which is widely used in the field of medicine and archaeology has been utilized in the field of civil and material engineering in order to generate realistic 3-D mesoscale analysis model for concrete, asphalt concrete, and other particulate materials and to overcome the drawbacks of the conventional regular shape particle mesoscale analysis model. The internal configuration of the X-ray CT equipment is illustrated in Figure 3.

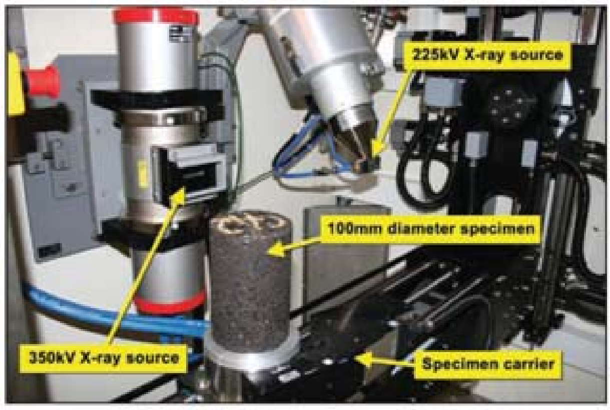
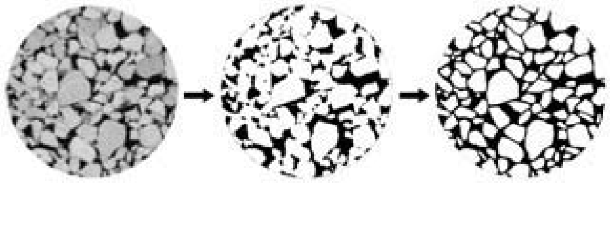


Figure 3. X-ray computed tomography (CT) for capturing material microstructure

The 3-D microstructure of the particulate material can be generated based on the real images obtained from the X-ray CT. For example, from the original 2-D X-ray CT image (Figure 4 (a)), the final 2-D image with well-separated aggregates (Figure 4 (c)) for constructing 3-D microstructure can be obtained via several filtering processes. White and black region, in Figure 4 (c), represents the aggregates and mortar matrix, respectively, and initial defects, such as initial cracks and voids are not considered for the simplicity in this example. These filtering processes may be done by hand one by one. However, it is a laborious

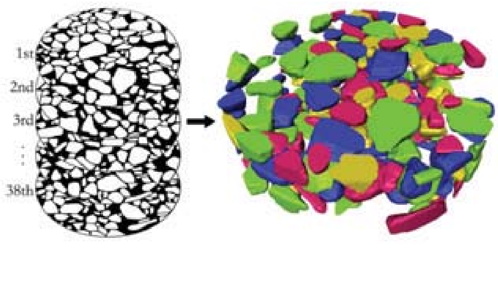


(a) (b) (c)

Figure 4. Image processing: (a) original image, (b) filtered image, and (c) image with well-separated aggregates

task, and it may not be possible to maintain consistency for all 2-D images. Therefore, commercial software (i.e. Avizo and Simpleware) is commonly used for the image filtering process.

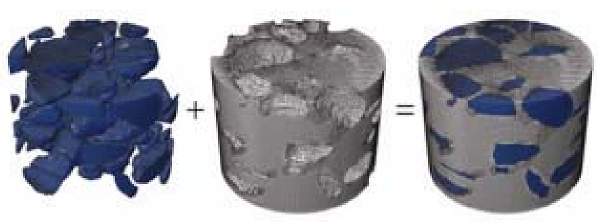
The commercial software, such as Avizo and Simpleware is also used to generate 3-D aggregate model from the filtered 2-D X-ray CT images. Figure 5 (b) shows the generated 3-D aggregates from the stacked 2-D images. The smoothness of the aggregate surface depends on the distance between the stacked 2-D images, and 38 2-D images are used to generate the 3-D aggregate model in this example. Furthermore, what is the most important in the series of 2-D and 3-D image processing is to isolate each aggregate from others in 3-D space in order to guarantee the independent movement of each aggregate from others and consequently to obtain more realistic simulation result from the 3-D mesoscale analysis.



(a) (b)

Figure 5. 3-D aggregate modeling: (a) stacked 2-D images and (b) generated 3-D aggregates

The generated 3-D aggregate model through the series of the image processing can now be exported to well-known commercial finite element (FE) software, such as Abaqus, Ansys, and LS-Dyna for the mesoscale FE simulation. Since the finite element meshing technique of the commercial image processing software is not satisfactory and limited yet, FE software is generally preferred to assigning mesh, and a series of the general FE modeling process can be done straightforwardly. Figure 6 shows the meshed 3-D mesoscale FE analysis model. It should be mentioned that the 3-D aggregate model generated through the image processing (Figure 5(b)) is cored and the actual size of the 3-D analysis model in Figure 6 is reduced here. As seen in Figure 6, a considerably fine mesh should be assigned to maintain the original shape of aggregates, consequently, a high-performance computing system is needed to simulate.



(a) (b) (c)

Figure 6. 3-D finite element mesh: (a) aggregates, (b) mortar matrix, and (c) concrete

In conclusion, it is obvious that the novel 3-D micro-mechanical modeling technique and simulation can be used more effectively for establishing the property-structure relationship and for identifying the key microstructure parameters for enhanced performance. Special emphasis of the 3-D mesoscale analysis model with actual shape particles is placed on investigating the true effects of particle shape and distribution as well as the effect of particle volume fraction on the overall behavior of material.

Furthermore, the 3-D micro-mechanical modeling of particulate material using X-ray CT images of the experimental specimen makes it possible to compare directly simulation results, such as the initiation and propagation of cracks, strain localization, and localized damage due to the environmental effect, such as moisture and heat with results obtained experimentally.

References

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