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KEYNOTE PAPER

SHAPE SIMULATION OF GRANULAR PARTICLES IN CONCRETE AND APPLICATIONS IN DEM

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ABSTRACT

Aggregate occupies at least three-quarters of the volume of concrete, so its impact on concrete's properties is large. The sieve curve traditionally defines the aggregate size range. Another essential property is grain shape. Both, size and shape influence workability and the mechanical and durability properties of concrete. On the other hand, the shape of cement particles plays also an important role in the hydration process due to surface dissolution in the hardening process. Additionally, grain dispersion, shape and size govern the pore percolation process that is of crucial importance for concrete durability

Discrete element modeling (DEM) is commonly employed for simulation of concrete structure. To be able doing so, the assessed grain shape should be implemented. The approaches for aggregate and cement structure simulation by a concurrent algorithm-based DEM system are discussed in this paper. Both aggregate and cement were experimentally analyzed by X-ray tomography method recently. The results provide a real experimental database, e.g. surface area versus volume distribution, for simulation of particles in concrete technology. Optimum solutions are obtained by different simplified shapes proposed for aggregate and cement, respectively. In this way, reliable concepts for aggregate structure and fresh cement paste can be simulated by a DEM system.

Keywords
Aggregate, concrete, DEM, shape, packing.

INTRODUCTION

A particle is defined as the smallest discrete unit of a powder mass that can not be easily subdivided [1]. The shapes of real particles are irregular, either from coarse aggregate or from mineral admixture in concrete. Aggregate occupies at least three-quarters of the volume of concrete, so its impact on concrete's properties is large. The sieve curve traditionally defines the aggregate size range. Another essential property is grain shape. Both, size and shape influence workability and the mechanical and durability properties of concrete. The definition of the actual grain shape as well as the representation in a discrete element modeling (DEM) system is complicated, however. Further, the real shape of aggregate or binder particles can vary widely. The sphere is therefore generally adopted in conventional simulation systems, despite imposing serious limitations.

The shape of cement particles plays also an important role in the hydration process due to surface dissolution in the hardening process. Additionally, grain dispersion, shape and size govern the pore percolation process that is of crucial importance for concrete durability [2]. Cement hydration in a DEM approach renders the possibility of investigating microstructure development and properties of concrete. A digital image-based model [3] as well as continuum models [4,5,6] have been developed for this purpose. Apart from the digital image-based model, particle shape is generally assumed spherical in such systems, because of inherent simplification in algorithm formulation; however, at the cost of possibly biased simulation results. Recently, some reference cement and aggregate were analyzed by micro-tomography (μCT) or X-ray tomography (CT) [7,8]. The results provide real experimental databases of aggregate and cement that yields valuable parameters for simulation in DEM. However, using real particle shapes in DEM is too expensive and (computer) time-consuming. In other words, it is not practical to model a large number of particles, each with its actual shape and size [9]. Therefore, choosing one or several shapes to represent different particles is a more practical way. Different simulation methods can be adopted for simulation of aggregate.

In this paper, simulation strategies for the representation of arbitrary-shaped aggregate and cement grains applied in concrete technology is presented. This simulation approach will be incorporated in a physical concurrent algorithm-based DEM system. A shape analysis study was also conducted with some simpler shape solutions for aggregate as well as cement grains, whereby the CT and μCT results served as references [7,8]. Based on this analysis, different simulation strategies are proposed as the preferred approaches to aggregate and cement particle simulation. The generation of the densely packed structure of aggregate and microstructure of fresh cement paste can be further conducted by using an advanced DEM system.

SHAPE SIMULATION OF AGGREGATE GRAINS

Generally, aggregate in concrete can be divided into two groups: gravel of fluvial origin and crushed rock, representing rounded and angular-shaped particles, respectively, as shown in Fig. 1 The ellipsoid was selected to represent the river gravel particles. On the contrary, the polyhedron was used for simulation of crushed rock grains. For efficiency of calculation in DEM, enough calculation nodes are necessary for every particle. Therefore, using a mesh is crucial for the generation of the particle.

A specific group of shapes with 4-8 facetted surfaces are developed to represent crushed rock, following Guo's field investigations [10]. This greatly simplifies the simulation of crushed rock since only the two parameters, *i.e.* sieve size and the maximum size of surface

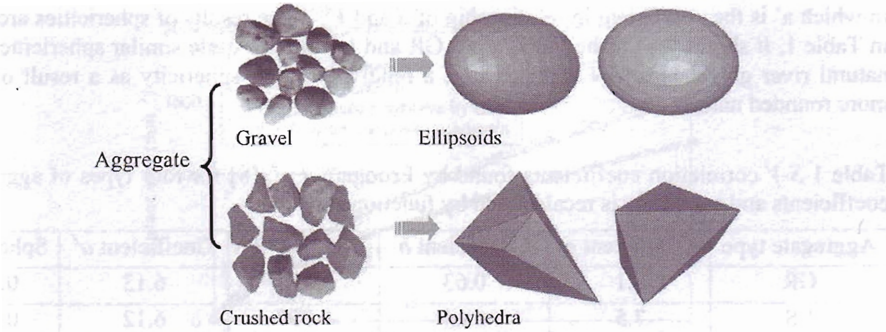


Fig. 1. Simulation strategy of arbitrary shaped aggregate; (top) differently shaped ellipsoids represent river gravel; (bottom) differently shaped polyhedrons represent crushed rock

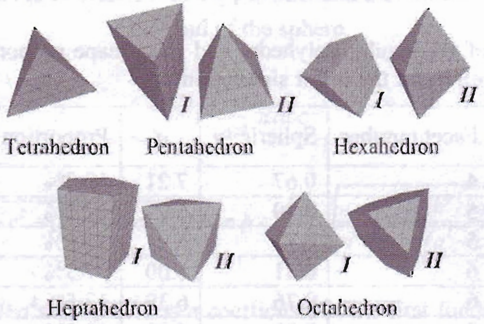


Fig. 2. Nine regular polyhedra with facet number 4~8

element, are required. Fig. 2 illustrates the meshed particles with different number of facets. The quantity proportions of each polyhedron in the whole group of crushed rock proposed by Guo [10].

Recently, in a study of Erdogan *et al.* [8], the shapes of four different types of aggregate, GR, LS, IN and AZ were investigated by the CT method and reconstructed by the spherical harmonic technique [8]. The most interesting information from their shape analysis is the surface area (S) vs. volume (V) information of each particle of different types of aggregate. A function $S=aV^b$ was used to regress the correlation of S and V in each type of aggregate [8]. The coefficients a and b were obtained for each type of aggregate as shown in Table 1 [8]. The variances of the regressions were all higher than 0.98.

As an ideal value of b in standard shapes is 2/3, the regression function $S=a'V^{2/3}$ was employed to fit different types of aggregate. For effective experimental conditions as to volume (<4000 mm^3) and size range, a' is determined for each type of aggregate with a variation lower than 5%, as shown in Table 1. The important shape index, sphericity, can be defined as the surface area ratio of the equivalent sphere (with equal volume) and the real particle. An approximate value for sphericity in each type of aggregate can as a consequence be calculated by

$$Sphericity = \frac{S_{eq.sphere}}{S_{particle}} = \frac{4\pi(\frac{3V}{4\pi})^{2/3}}{a'V^{2/3}} = 4.836(a')^{-1} \quad (1)$$

in which a′ is the coefficient in relationship of S and $V^{2/3}$. The results of sphericities are listed in Table 1. It shows the crushed rock types GR and LS to have quite similar sphericities. The natural river gravel types IN and AZ have a relatively larger sphericity as a result of their more rounded nature.

Table 1 S-V correlation coefficients found by Erdogan *et al.* [8] for four types of aggregate; coefficients and sphericity is recalculated by function $S=a'V^{2/3}$

Aggregate type	Coefficient a	Coefficient b	Variance R^2	Coefficient a'	Sphericity
GR	8.1	0.63	0.99	6.13	0.79
LS	7.5	0.64	0.997	6.12	0.79
IN	8.6	0.62	0.99	6.06	0.80
AZ	9.1	0.61	0.98	5.95	0.81

Table 2 Shape indices of the regular polyhedra and each shape proportion proposed by Guo [10] and a revised proportion for the better simulation

Shapes	Facet number	Sphericity	a'	Proportion by Guo	Revised proportion
Tetrahedron	4	0.67	7.21	10.0%	5%
Pentahedron I	5	0.70	6.95	12.5%	5%
Pentahedron II	5	0.72	6.71	12.5%	5%
Hexahedron I (Cube)	6	0.81	6.00	17.5%	10%
Hexahedron II	6	0.76	6.39	17.5%	10%
Heptahedron I	7	0.83	5.83	10.0%	15.5%
Heptahedron II	7	0.80	6.06	10.0%	15.5%
Octahedron I	8	0.85	5.72	5.0%	17%
Octahedron II	8	0.78	6.24	5.0%	17%
Sphere	∞	1.00	4.84	-	-

The proposed shapes by Guo [10] for simulation of crushed rock are then analyzed with experimental results of Erdogan *et al.* [8]. Shape indices of different regular polyhedra are listed in Table 2 with the sphere as a reference. It demonstrates that the shape indices of crushed rock samples GR and LS are within the range of shape indices of these nine regular polyhedra. Guo [10] also proposed from his experimental investigation for crushed rock a proportion of each shape category, as listed in Table 3. Next, the composite polyhedra method proposed by Guo [10] can be compared with experimental results of GR and LS [8], shown in Fig. 3. Generally speaking, Guo's proposal fits the data of aggregates GR and LS quite well. But there is some deviation in the large particle range. Therefore, a better proportion of each category is proposed shown in Table 1 as well as in Fig. 3. By theses proportions, S-V information of composite polyhedra can better comply with the experimental results of GR and LS types. By this simplified simulation, the crushed rock structure in concrete can be properly represented with DEM as surface area is important for the mechanical properties of concrete and for the ITZ proportion that influences the transport properties.

Ellipsoids are particularly interesting because with only 3 parameters a variety of shapes, ranging from oblate to oblong can be described. Three principal axes (a represents longest, b medium size and c shortest axis) determine the shape of an ellipsoid. By parameter variation, different ellipsoids with different S-V relationships can be derived. V and S can be obtained by

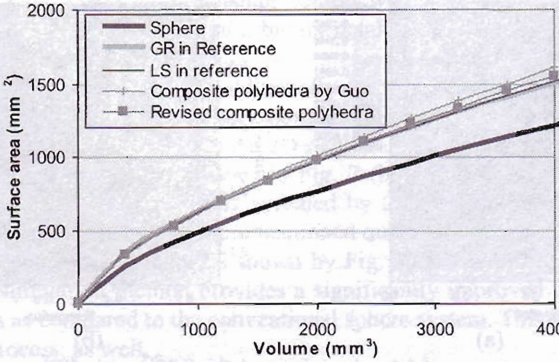


Fig. 3. *S-V* curves of crushed rock types (GR and LS), of composite polyhedra and of the sphere

equations from [11]:

$$V = \frac{4}{3}\pi abc \tag{2}$$

$$S = 2b\sqrt{2}\int_0^{\pi}\sqrt{a^2+c^2+(a^2-c^2)\cos(2\phi)}\sin\phi \times E\left(\frac{c}{b}\sqrt{\frac{2(b^2-a^2)}{a^2+c^2+(a^2-c^2)\cos(2\phi)}}\sin\phi\right)d\phi \tag{3}$$

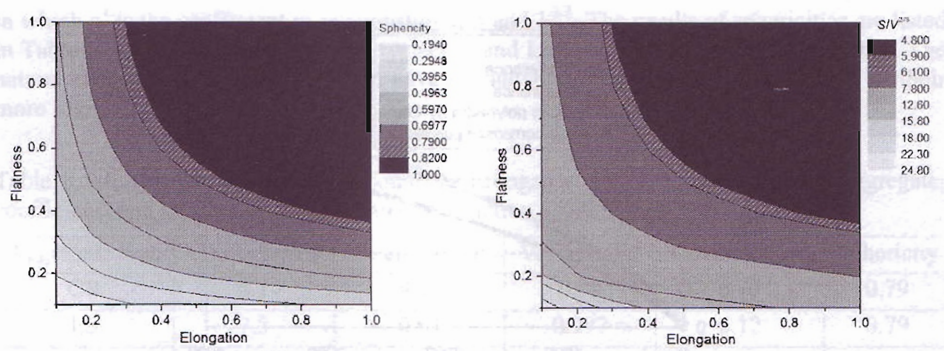
in which, $E=(b^2\cos^2\theta+a^2\sin^2\theta)\sin^2\theta$ is a coefficient of the first fundamental form and θ is a polar angle. Flatness and elongation are defined as c/b and b/a, respectively. So, the distribution contours of sphericity and $S/V^{2/3}$ (or a') with different elongation and flatness values can be constructed, as depicted in Fig. 4.

Figure 4 (a) reveals that if elongation and flatness are both larger than 0.5, sphericity of an ellipsoid will be close to 1. $S/V^{2/3}$-contours with elongation and flatness are plotted in Fig. 4(b). With experimental values of JN and AZ types in Table 1, the hatched regions in Fig. 4 can be selected as the optimum solution. The preferred elongation and flatness of an ellipsoid should exceed 0.3 and 0.4, respectively. This conclusion is comparable with the experimental results on gravel in Fig.4. The selected ellipsoids are thus neither very elongated nor flat.

SHAPE SIMULATION OF CEMENT GRAINS

Computer X-ray micro-tomography offers a potential solution for shape assessment of cements, as shown by Garboczi and Bullard [7] and by Bullard and Garboczi [12]. The microstructures of hydrated cements based on actual grain shape and on spherical shape were found significantly different in this study. The results provide an experimental database of this cement that yields some valuable parameters for DEM simulation of cement hydration.

Using grains in numerical simulation similar to the real ones would be too expensive. So, it is crucial finding simpler shapes that are sufficiently representative. Similar as in the case of the aggregate simulation, a shape analysis study was therefore conducted with some simpler shapes. Based on this analysis, a simulation strategy is proposed for cement. More realistic but still cost-effective particle shapes should therefore be implemented in DEM systems.



(a) (b)

Fig. 4. Distribution contours of (a) sphericity and (b) $S/V^{2/3}$ with different elongation and flatness of an ellipsoid

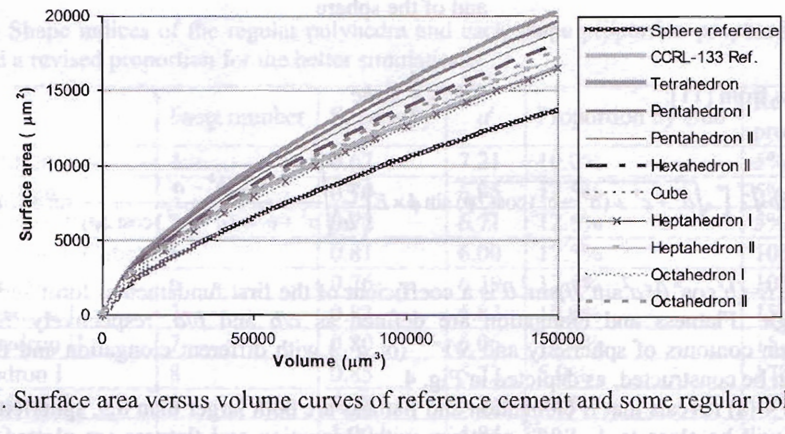


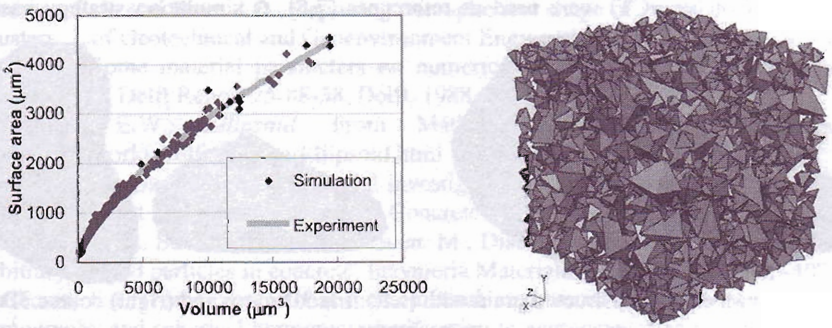
Fig. 5. Surface area versus volume curves of reference cement and some regular polyhedra

Cement is made by raw materials such as limestone, clay, etc., after a process of calcinations. Raw cement clinkers are hard, large and roughly rounded particles on a scale of centimeters. Raw cement clinkers are ground in the miller with a small amount of gypsum into small cement grains. Hence, shape of final cement grains are tended to angular shapes on a scale of micrometers. Polyhedra seem more reasonable for simulation of cement grains based on this consideration. Nine polyhedra in Fig. 2 are also selected for this shape analysis. As the surface area-to-volume (*S-V*) relationship was the most important information obtained from the experimental reference [7], values of these shape indices are plotted in Fig. 5. The surface over volume *S-V* relationship can generally be also expressed by $S=a'V^{2/3}$. Within an effective experimental volume of 10,000~150,000 μm^3 [7], coefficient a'=5.8 was found by regression analysis, with a coefficient of variation lower than 5%. Proposed shapes should therefore approximate this value. In this case, sphericity can be calculated as 0.83.

From Fig. 5 and Table 2, it is concluded that the heptahedron *I* and the octahedron *I* offer the most promising solutions. The octahedron is selected for the simulation study because of allowing an easier transformation into irregular shapes by parameter variation. Three axes can be employed for this purpose, as in [13]. Since the *S-V* curve of an octahedron is close to that of the reference cement, some limited random variation can be applied accounting for the diversity of particle shape.

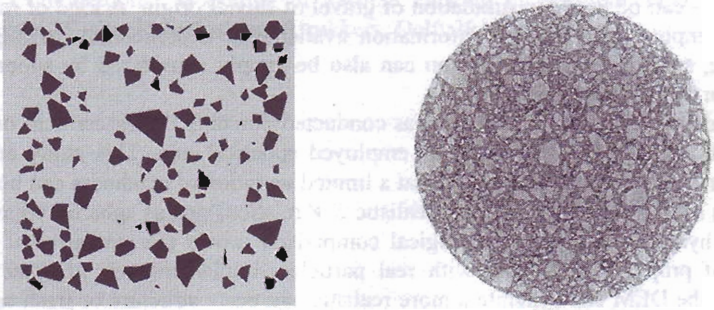
Figure 6(a) shows the *S-V* distributions of randomly generated octahedra with an experimental reference curve. This Figure reveals the cases of 1000 particles with longest axis in 10~50 μm size range. The *S-V* relationships comply well with experiments. Fig. 6(b) shows an example of a loose packed structure of arbitrary octahedrons supposedly representing fresh cement.

Morphological comparisons can additionally be made between sections of simulated particle structures and of real ones. As an example, Fig. 7(a) shows a random section of the simulated structure shown in Fig. 6(b) and a 2D section of a real cement structure obtained by X-ray micro-tomography. Cement particles in Fig. 7 (b), displayed in light grey, obviously reveal the angular shape that is similarly revealed by the section of the polyhedral cement particles in Fig. 7(a). This adds to the aforementioned quantitative matching of *S-V* features of real and simulated cement structures, as shown by Fig. 6(a). Therefore, it can be concluded that the proposed simulation method provides a significantly improved option for modelling of cement particles as compared to the conventional sphere system. This will also have impact on the hydration process, as well.



(a) (b)

Fig. 6(a) Computer simulation of 1000 particle in 10~50 μm size range and experimental regression results [7] and (b) visualized structure of compacted grains



(a) (b)

Fig. 7(a) section of the simulated structure (1000 octahedron grains in 10~50 μm size range); (b) 2D section of a real fresh cement structure (Cement-133) obtained by X-ray micro-tomography; w/c=0.35. Source: http://visiblecement.nist.gov/cement.html.

DISCUSSION AND CONCLUSIONS

Particles used in concrete, either aggregate, cement or minerals, have irregular shapes. The definition or simulation of shape is therefore inevitably complex. Reconstruction of an irregular shape is technically possible, especially with development of CT (or μCT) and SH [7,14]. Even with traditional 3D image analysis, an irregular particle shape can roughly be reconstructed by combining the vertical and horizontal profiles with a 3D mesh program [15,16]. Examples are plotted in Fig. 8. Using a large amount of grains in numerical simulation that are similar as the real ones would be too expensive as to equipment and computer time [9]. So, it is crucial finding simpler shapes that are sufficiently representative. Nevertheless, a spherical particle shape normally assumed in conventional simulation systems is at the cost of possibly biased simulation results [12].

Therefore, a shape analysis study was conducted with some simpler shapes for simulation of aggregate as well as of cement. The shape information of real aggregate and cement by CT or (or μCT) were used as references [7,8]. A simulation strategy based on

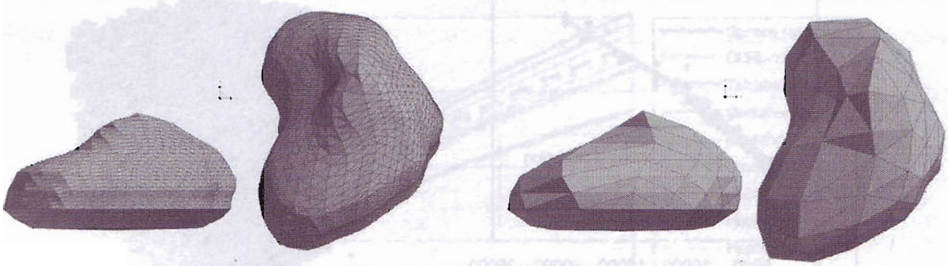


Fig.8. Two views of a reconstructed grain with (left) fine 3D mesh and (right) coarse 3D mesh, respectively.

different origins of arbitrary-shaped aggregate grains is proposed. Composite polyhedra with nine proposed simple shapes [10] can properly represent the crushed rock used in concrete. This method can better comply with the *S-V* correlations extracted from experimental findings [8]. Ellipsoids can be used for simulation of gravel of fluvial origin. A kind of relatively flat ellipsoids complies with the *S-V* information available in experimental investigations [8]. Furthermore, surface texture simulation can also be simply considered by superimposing a sine function on a regular shape [16].

For hydration simulation, a study was conducted pursuing the assessment of physically more realistic shapes as the commonly employed spherical one. This study encompassed polyhedra and ellipsoids. It was shown that a limited variation of octahedra can be considered an optimum solution. They offer more realistic *S-V* relationships as spheres, which is crucial for cement hydration, [12]. Morphological comparison shows the similarity of the packed structures of proposed polyhedra with real particles. Implementation of these simulation strategies in the DEM can generate a more realistic aggregate structure or fresh cement paste in concrete technology.

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