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THE 'SIGNATURE' OF PARTICLE GEOMETRY - DEM MODELLING PERSPECTIVE

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Abstract. This study evidences that the particle surface-area-to-volume ratio (A/V) and the particle volume (V) have the key information of particle geometry and the 'signature' is realized by a power-law relationship between A/V and V in a form of $V = (A/V)^{\alpha} \times \beta$. We find that the power value α is influenced by the shape-size relationship while the β^* term (β evaluated with a fixed value of $\alpha = -3$) informs the average particle shape of a granular material regarding the overall angularity. This study also discusses how the particle shape can be retrieved in terms of Wadell's true sphericity using the A/V and V. This concept is linked to another shape index M that interprets the particle shape as a function of surface area A, volume V, and size L. This paper explains the analytical aspects of geometric 'signature' and examines the idea using the example particles to address the DEM modelling-related questions.

1 INTRODUCTION

With the recent advances in computing resources and modelling techniques, the discrete element method (DEM) has evolved to consider realistic particle geometry for more accurate interactions between particles. Therefore, the simulation fidelity of granular material behaviour could have been greatly enhanced. However, when it comes to modelling of mineral particles (e.g., for a geomechanics problem), a large gap still exists with many questions that remain to be better answered. For example, every mineral particle looks different in terms of shape and size, then how can we model these different particles for DEM analysis? If it is impractical to model all of those, how many shapes do we need to model to make DEM simulation as accurate as possible? Is there a systematic way we can use to identify some representative shapes for DEM modelling? In general, the particle shape changes with size, then how can we effectively model this?

Furthermore, the particle shape effect on the granular material behaviour is a fundamental research topic for which DEM has been broadly adopted. However, we need to look at the 'shape effect' a little more carefully because the shape effect cannot be isolated. The 'particle shape' is indeed a comprehensive term, thereby being a function of the coupled geometry parameters (i.e., volume, surface area, and size). Thus, the effect of 'particle shape' can be triggered by any of geometry parameters. For example, Figure 1a is a cube, and Figure 1b is a rectangular prism whose length is twice longer than the cube in Figure 1a. The aspect ratios are different, but the volume of Figure 1b is also twice larger than Figure 1a. Then, if these particles are used for the shape effect study using DEM, how can we isolate the effect of different aspect ratios from the effect of different volumes? The rectangular prism can be scaled to Figure 1c to have the same volume as the cube, but these particles (Figure 1a and c) still have different surface areas and sizes as well as different shapes. Therefore, what we studied using DEM was not the particle 'shape effect' but the particle 'geometry effect' where the shape is one of the main contributing factors (that cannot be isolated) to the granular material behaviour. Nevertheless, the 'particle shape' is a comprehensive term, how can we describe the shape in terms of other geometry parameters? This study finds the particle surface-area-to-volume ratio (A/V) and the particle volume (V) can be used to describe the shape and are the key information to reveal the 'signature' of particle geometry.

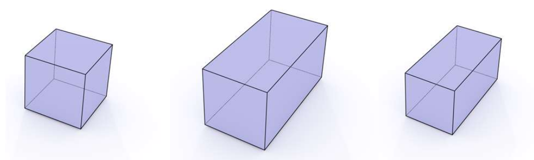


Figure 1. Example of particle geometry variation for the shape effect study; (a) Cube; (b) Rectangular prism with L:W = 2:1; and (c) A smaller rectangular prism having the same volume with the cube in (a)

2 M-A-V-L VS. WADELL'S TRUE SPHERICITY

A new concept M-A-V-L was introduced by Su et al. [1] with Equation (1) that translates the 3D particle morphology (shape) M as a function of surface area A, volume V, and size L, where L is defined by the diameter of particle's circumsphere (colloquially, circumdiameter). We recently found that the principle was implicitly embedded in Wadell's 'true' Sphericity proposed about a century ago [2] although the original definition was never discussed that way in the granular materials research community.

$$M = A/V \times L/6 \quad (1)$$

Wadell proposed the 'true' Sphericity S to quantify the 3D particle shape and defined it as the ratio between two surface areas as shown in Equation (2) comparing the particle surface area A with the surface area of the reference sphere A_s. The reference sphere has the volume V_s same with the volume V of the particle (i.e., $V_s = V$).

$$S = A_s / A \quad (2)$$

While the original definition in Equation (2) is well-known, the granular materials research community has not recognized that S can be reformulated as a function of surface area A, volume V, and size D as shown in Equation (3), where S^{-1} is the inverse of S. The size D is the diameter of the reference sphere having the same volume V with the particle. Therefore, as shown in Equation (4), D can be computed from V using the analytical relation between sphere diameter and volume.

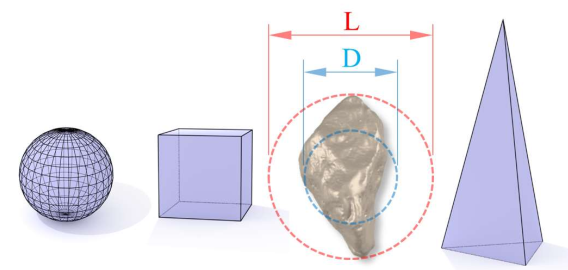
$$1/S = S^{-1} = A/V \times D/6 \quad (3)$$

$$D = 2\times(3V/(4\pi))^{1/3} \quad (4)$$

There is a similarity as well as the difference between M and the true Sphericity, S. Equations (1) and (3) are written in a similar form except for the length term: L for Equation (1) and D for Equation (3). This means that both indices similarly interpret the 3D particle shape as a function of surface area, volume, and size. The difference is how the size is determined. S^{-1} is evaluated using the diameter D of the reference sphere having the same volume V with particle. Therefore, D is certainly redundant information because it can be derived from V as shown in Equation (4). However, the index M considers L (i.e., circumdiameter) in the place of D. Therefore, M complements S^{-1} with the additional parameter L. Comparing Equations (1) and (3), the M/S^{-1} ratio (or simply M×S) is the ratio of L/D as shown in Equation (5) which can distinctively informs shape elongation.

$$M/S^{-1} = M\times S = L/D \quad (5)$$

Figure 2 shows an example. All particles in the figure have the same D (=1.24 mm) because the volumes of all particles are set to 1 mm^3. However, L is different because it considers the length to the farthest corner of the particle. Figure 2c schematically shows how L and D are evaluated. The sphere has the smallest S^{-1} and M values which are 1. Both shape index values increase with elongation and angularity in order of sphere, cube, the mineral particle, and elongated tetrahedron. The point is that it is hard to differentiate the contribution of elongation from that of angularity to the shape by looking at either S^{-1} or M. However, comparing S^{-1} and M gives useful information about elongation. While both (b) cube and (c) the mineral particle have comparable S^{-1} values, (c) has a significantly higher M compared to (b) due to the elongation. This is reflected in the higher M/S^{-1} value of (c) compared to (b). The M/S^{-1} value can be even higher with more elongation as shown for the (d) elongated tetrahedron.



	(a)	(b)	(c)	(d)
Volume (V):	1.00 mm^3	1.00 mm^3	1.00 mm^3	1.00 mm^3
Surface area (A):	4.84 mm^2	6.00 mm^2	6.24 mm^2	7.97 mm^2
Size (D):	1.24 mm	1.24 mm	1.24 mm	1.24 mm
Size (L):	1.24 mm	1.73 mm	2.18 mm	3.33 mm
S^{-1}:	**1.00**	**1.24**	**1.29**	**1.65**
M :	**1.00**	**1.73**	**2.27**	**4.42**
M/S^{-1} (= L/D):	**1.00**	**1.39**	**1.76**	**2.68**

Figure 2. Particle shape evaluated in terms of S^{-1} and M; (a) Sphere; (b) Cube; (c) a 3D-scanned mineral particle; and (d) Elongated tetrahedron

3 POWER-LAW BETWEEN A/V AND V

As discussed in the previous section, the individual particle shape can be described in terms of the true Sphericity using A/V. In addition, A/V can be useful to describe the 'signature' of particle geometries at the granular material level such as (i) the shape-size relation and (ii) the overall angularity. The relation between A/V and V of particles can be approximated with a 'power-law' [3] in a form of Equation (6). Considering this power-law relation is presented as a linear plot in the log-log space as shown in Equation (7), the power value α represents the slope of the log-log plot, and the term β represents the plot's intercept at A/V = 1.

$$V = (A/V)^{\alpha} \times \beta \quad (6)$$
$$\log(V) = \alpha \times \log(A/V) + \log(\beta) \quad (7)$$

Figure 3 shows an example, where the A/V and V values of three groups of particles are presented. Each group is composed of 15 particles of sphere, cube, or tetrahedron. The power law relations are plotted in a log-log scale with the α and β values presented. As shown in the figure, the power value α (slope) is invariantly -3 for particles having a same shape, indicating the shape does not change with size. If all 45 particles are considered as a group, the estimated power value α is still -3 as shown with the black dotted line in the figure. Likewise, α = -3 indicates the shape distribution does not change with size, i.e., there is no shape-size relation. The β value is the intercept at A/V = 1 in the regression analysis, while β* indicates the intercept with a fixed value of α = -3. In this example, β* = β because the power regression is realized with α = -3, but β* ≠ β if the slope α is different from -3 in the regression analysis (e.g., Figure 5 to be discussed later). Hereafter, β* is considered in this paper to demonstrate β* can represent the average particle shape of a granular material regarding the overall angularity. As shown in the figure, β* is 113.09 for spherical particles, β* is 216 for cubes and β* is 374.12 for tetrahedra with α = -3, inferring that the β* increases with the angularity of particle geometry.

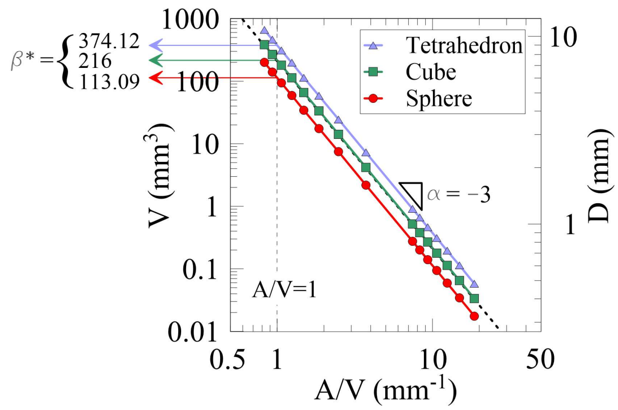
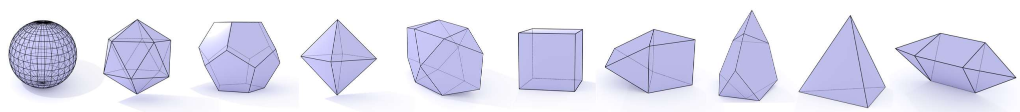


Figure 3. Examples of power-law for the three groups of identical shape (spheres, cubes, and tetrahedrons)

Then, what if there are different particle shapes mixed? Let us consider the example in Figure 4 to see how α and β* values are obtained. Two groups of particles are considered with various elongations and angularities. These particles are theoretical solids, so the detailed information of geometry can be found in existing literature including Mathematica's polyhedron library [4]. Icosahedron, dodecahedron, octahedron, cube, and tetrahedron are the Platonic solids. On the other hand, bilunabirotunda, gyrobifastigium, augmented tridiminished icosahedron (ATI), and elongated triangular dipyramid (ETD) are selected from the Johnson solids. Both groups have the same set of 10 different shapes, of which total volume of each group is identical. The evaluated S^{-1} and M values are shown in the figure, where the ETD is shown the most elongated and angular per the indices. The main difference between the two groups is the shape-size relation. In Group #1, the size D increases with shape angularity and elongation (from the left to the right in the figure). The sphere, therefore, has the smallest size (D = 0.5 mm) and D increases with S^{-1}. On the other hand, the size D in Group #2 decreases with increase of S^{-1}, so the sphere is the largest in the group (D = 5.0 mm). The size L is not presented in the figure, but it can be easily computed by $L = D \times M/S^{-1}$.



	Sphere	Icosa-hedron	Dodeca-hedron	Octa-hedron	Biluna-birotunda	Cube	Gyrobi-fastigium	ATI*	Tetra-hedron	ETD**
S^{-1}:	**1.00**	**1.06**	**1.10**	**1.18**	**1.20**	**1.24**	**1.30**	**1.36**	**1.49**	**1.51**
M :	**1.00**	**1.26**	**1.26**	**1.73**	**1.86**	**1.73**	**2.21**	**2.42**	**3.00**	**3.67**
M/S^{-1} (= L/D):	**1.00**	**1.18**	**1.15**	**1.46**	**1.55**	**1.40**	**1.69**	**1.78**	**2.01**	**2.43**
D (Group #1):	0.50	0.60	0.70	0.80	0.90	1.00	2.00	3.00	4.00	5.00
D (Group #2):	5.00	4.00	3.00	2.00	1.00	0.90	0.80	0.70	0.60	0.50

ATI* : Augmented Tridiminished Icosahedron
ETD** : Elongated Triangular Dipyramid

Figure 4. Two particle groups with the opposite shape-size relation; The unit of length is mm.

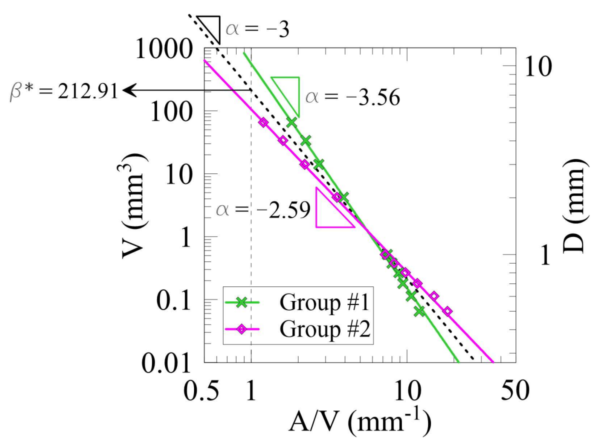


Figure 5. Power-law relation between A/V and V for Group #1 and #2

The power-law relation between A/V and V is shown in Figure 5. The slope α from the regression analysis indicates the important information regarding the relation between shape and size of particles. Considering α = -3 presents no shape-size relation (i.e., a reference), α < -3 (steep slope) indicates that smaller particles tend to have a more spherical and rounder shape than the larger particles. On the other hand, α > -3 (gentle slope) indicates the opposite, i.e., larger particles tend to be more spherical and rounder. This shape-size relation is evidenced with the plots in the figure, i.e., α = -3.56 (steep slope) for Group #1, and α = -2.59 (gentle slope) for Group #2. The black dotted line $\alpha = -3$ is shown in the figure as the reference. The β^* value is computed with α set to -3, and the average log(A/V) and the average log(V) obtained from the data points are used in Equation (7). The β^* value can be interpreted as the average shape index for a group of particles. The evaluated β^* is commonly found to be 212.91 for each Group #1 and #2, because the constituent shapes in these groups are identical. The β^* value is close to that of cubes-only group (Figure 3), informing the overall angularity of the particle shapes is close to the cube's.

4 CONCLUDING REMARKS

This paper discusses a new perspective regarding how particle shape, volume, surface area, and size are related, and characterizes the relation at two different levels - (i) individual particle level, and (ii) particle group level (i.e., granular material).

(i) The shape of an individual particle can be interpreted as a function of surface area A, volume V and size L. The $M = A/V \times L/6$ concept introduced by Su et al. [1] is revisited in this paper and compared with Wadell's true Sphericity S. This paper uncovers the $S^{-1} = A/V \times D/6$ concept that similarly characterizes the 3D particle shape as a function of the other geometry parameters. This paper finds the value of M/S^{-1} provides useful information about elongation.

(ii) The shape-size relation and average shape index of particles can be understood using a 'power-law' between A/V and V. This 'signature' of the particle geometries is realized as a linear plot in log-log space. The power value α (slope of the plot) in the unconstrained regression analysis indicates the shape-size relation, and the intercept term β^* (evaluated by the constrained analysis with $\alpha = -3$) represents the overall angularity of the particle shapes. Furthermore, the A/V and V space allows for presenting the particle volume, surface area, and size, which enables to comprehensively characterize the particle geometries.

The findings will allow for more effective particle geometry modelling in DEM. In general, there are too many particle shapes that exist in a naturally occurring granular material. Not all shapes can be modelled for DEM analysis, and therefore some representative shapes need to be identified for the particle modelling. However, it has been always unclear to determine what shapes are typical or dominant. Furthermore, the selection of such shapes has been somewhat subjective in DEM modelling community. The identified α and β^* information will help systematically model the DEM particles.

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