A New Interpretation of Three-Dimensional Particle Geometry: M-A-V-L

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ABSTRACT

This study provides a new interpretation of 3D particle geometry that unravels the ‘interrelation’ of the four geometry parameters, i.e., morphology M, surface area A, volume V, and size L, by proposing a new formula, $M = A/V \times L/6$, which translates the 3D particle morphology as a function of surface area, volume, and size. The $A/V \times L$ of a sphere is invariantly 6, thus M indicates a relative morphological irregularity compared to the sphere. The minimum possible value of M is clearly one, and may range to approximately three for typical coarse grained mineral particles based on the Krumbein and Sloss chart. This paper also demonstrates how the proposed formula can be leveraged to systematically describe the distributions of the interrelated 3D particle geometry parameters, M-A-V-L, which would be useful to predict the mechanical property of granular materials. Therefore, this new approach will help robustly relate the particle scale geometric information to the macroscopic property of granular materials.

Keywords: Interrelated 3D Particle geometry; Morphology; Surface area; Volume; Size;

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1 INTRODUCTION

The granular materials are prevalent in nature such as soil, and important in many industries including construction, agriculture, pharmaceutical, and others, which are known as the second-most manipulated material (Richard et al., 2005). The influence of particle geometry is a key to understand the complex behavior of the granular materials, but our knowledge of the subject remains at best incomplete. The systematic understanding of the geometry influence requires to effectively unravel the ‘interrelation’ of the four 3D particle geometry parameters, i.e., morphology M, surface area A, volume V, and size L, because the interrelation makes hard to independently discuss the influence of one geometry parameter from the other parameters. In other words, isolating one variable from the others is practically challenging. For example, if two different shaped particles are modeled while keeping the volume same, these particles inevitably get different particle sizes and surface areas from each other as illustrated in Figure 1a. Therefore, if these two particle models are adopted to study the different morphology effect in particle-based simulations (e.g., discrete element method), the different size and surface area also come into additional or uncontrolled effects on the behavior of granular materials. On the other hand, if the particle size is maintained from Figure 1a, these particles get different volumes and surface areas as well as the morphology (Figure 1b). While existing studies in the granular materials research mostly focused on either particle morphology or size effect, the particle volume is also an important factor that needs to be systematically considered as it is the major parameter that determines the granular skeletal (i.e. bulk) density. The particle surface area is another important factor, e.g., soil plasticity is greatly influenced by the surface area (Santamarina and Cho, 2004). The surface-area-to-volume ratio is a critical factor for estimating the performance of cemented granular materials (e.g., concrete) due to its direct impact on the quantity of bonding characteristics (a.k.a. “weak links”) at the interface of particle surface and binding matrix (Neville, 1996; Mindess, Young and Darwin, 2003; Wong et al., 2009; Mehta and Monteiro, 2013; Lee et al., 2018). On the other hand, the size scaling does not make any change to the morphology but still changes the volume and surface area (Figure 1c). These examples commonly demonstrate that these four 3D particle geometry parameters are interrelated and imply the morphology M may be interpreted as a function of the other three geometric parameters, i.e., surface area A, volume V, and size L, and vice versa. However, to the best of authors’ knowledge, no study to date has systematically investigated the interrelation of M-A-V-L.
Figure 1. Interrelated 3D particle geometry parameters; (a) Two different particle morphology with the same volume, consequently the particles have different sizes and surface areas. The size is measured in terms of the diameter of bounding sphere (shown as red circles); (b) Two different particle morphology with the same size, thus the particles have different volumes and surface areas; (c) Two different particles with same morphology having different volumes, surface areas, and sizes.

The concept of volume, surface area, and size of particles is straightforward, which can be defined by a single scalar value for each. On the other hand, the morphology has been traditionally characterized using three factors defined at three different scales: (i) global form (at large scale), (ii) local angularity (at intermediate scale), and (iii) surface texture (at small scale) as shown in Figure 2. The (i) global form provides the largest scale morphological information related to the particle’s diameter scale $O(d)$ and characterizes the extent to how equidimensional the particle morphology is. The (ii) local angularity describes the overall sharpness of corners defined at a length scale smaller by one order of magnitude $O(d/10)$ (Jerves, Kawamoto and Andrade, 2016). Sphericity and Roundness (Wadell, 1935) are the broadly adopted descriptors to optically characterize the global form and the local angularity. Both Sphericity and Roundness range between 0 and 1. A low Sphericity indicates an elongated shape such as ellipsoid, while a high Sphericity close to 1 indicates a near-equidimensional shape such as sphere; a low Roundness close to 0 indicates a particle with sharp corners, while a high Roundness indicates the opposite. In addition, Regularity is defined as the average of Sphericity and Roundness (Cho, Dodds and Santamarina, 2006), which can be leveraged to comprehensively describe the global form and the local angularity. The effect of (iii) surface texture has been mechanically characterized and modeled in terms of the inter-particle friction angle (Rowe, 1962; Lee and Seed, 1967; Terzaghi, Peck and Mesri, 1996) in the discrete element analysis (Lee, Hashash and Nezami, 2012; Huang et al., 2014).
Sphericity and Roundness are conventionally defined in 2D using the particle projection images (Zheng and Hryciw, 2015). These 2D descriptors have been commonly adopted due to the ease of characterization of the global form and the local angularity, but which have an inherent limitation to interrelating the morphology with the other 3D particle geometry parameters such as volume and surface area. While there is a 3D concept known as ‘true’ Sphericity that characterizes the global form of a particle by comparing its surface area to that of a sphere with the same volume (Wadell, 1935), there is no well-established 3D definition of ‘true’ Roundness due to the difficulty of characterizing the local angularity in 3D. Therefore, the existing 3D approach has a limitation in the local angularity quantification.

The objective of this study is to introduce a new formula that can systematically quantify the interrelation of the 3D particle geometry parameters, i.e., morphology M, surface area A, volume V, and size L, which will in return help better understand their concerted influence on the behavior of granular materials. While the robust characterization of surface texture is also of great importance, this study limits its scope on the morphology at the large and intermediate scales, because the small-scale surface texture would have relatively insignificant interrelation with volume, surface area, and size compared to the global form and the local angularity. For example, two identically shaped particles except the surface texture can be reasonably assumed to have the same volume, surface area, and size.

2 PROPOSED FORMULA FOR THE NEW INTERPRETATION

This study leverages the fundamental geometric principle: ‘morphology is related to surface-area-to-volume (A/V) ratio.’ An example is shown in Figure 3, where the A/V ratios are compared for the four different particle models having a same unit volume. The sphere has the ‘smallest’ A/V
ratio, which increases with more angular morphology. The A/V ratio of a cube is 1.24 times higher than that of a sphere with the same volume. The A/V ratio of a regular tetrahedron (which is more angular than the cube) is 1.49 times higher than the sphere. The A/V ratio also increases with elongation. The A/V ratio of a stretched tetrahedron in the figure is 1.65 times higher than the A/V ratio of the sphere with the same volume.

![Figure 3. Morphology related to surface-area-to-volume (A/V) ratio](image)

| Shape                  | A/V   | (A/V) / (A_s/V_s) |
|------------------------|-------|-------------------|
| Sphere (Round)         | 4.84  | **1.00**          |
| Cube (Angular)         | 6.00  | 1.24              |
| Regular tetrahedron (More angular) | 7.21  | 1.49              |
| Stretched tetrahedron* (Most angular w/ elongation) | 7.97  | 1.65              |

While the A/V ratio is related to particle morphology, it is critical to note that the ratio is not constant for a given morphology because the value depends on the size as implied by its unit, which is reciprocal length (L²/L³ = L⁻¹). Therefore, the A/V ratio is inversely proportional to the size. For this reason, the product of A/V ratio and size turns out to be an invariant for a given morphology, which therefore can be leveraged as a morphology indicator. Building upon this concept, this study proposes a new formula (Equation 1) that interprets the 3D particle morphology M as a function of the other geometry parameters, i.e., surface area A, volume V, and size L:

\[ M = \frac{(A/V \times L)}{(A_s/V_s \times L_s)} = \frac{(A/V \times L)}{6} \quad (1) \]

where the A/V ratio is multiplied by L for the scale-independent characterization of a given particle morphology, which is unit-less. The subscript s in Equation 1 means sphere. Therefore, M indicates the relative morphological irregularity compared to the sphere. The A/V×L does not change for a given morphology and A_s/V_s×L_s (of sphere) is invariantly 6. Therefore, the minimum possible value of M is clearly 1, and is higher than 1 for typical mineral grains. Further, the 3D information...
of the particle morphology is represented by a single scalar value. Figure 4 demonstrates an example, in which three different spheres (Figure 4c, d, and e) are scaled to match one of V, A, or L of the irregular particle in Figure 4b (highlighted in gray). The 3D model of the irregularly shaped particle is a polyhedron with 10374 triangular faces in its surface mesh, which is developed from a mineral grain using a photogrammetry technique introduced in Zhang et al. (2016). A larger particle with the same irregular morphology is also shown in Figure 4a, which is 1.5 times larger than the particle in Figure 4b size-wise. The volume and surface area of the particles in Figure 4a and b are numerically obtained from the developed 3D polyhedron model after scaling the size to 2.25 and 1.5 cm, respectively.

![Figure 4](image)

Figure 4. 3D morphology (M) translated as A/V×L/6; the size is measured in terms of the diameter of bounding sphere (shown as red circles).

Following observations can be made: (i) Particle morphology is related to A/V ratio, thus the irregular particle in Figure 4b has a higher A/V ratio compared to the sphere of the same L in Figure 4c, (i.e., 7.28 cm⁻¹ vs. 4 cm⁻¹); (ii) Since the A/V ratio is inversely proportional to the size, the A/V ratio increases while L decreases. For example, the A/V ratio of sphere in Figure 4e is larger by 1.5 times compared to that in Figure 4c (i.e., 6 cm⁻¹ vs. 4 cm⁻¹), while L is smaller by 1.5 times (i.e., 1.0 cm vs. 1.5 cm). This principle also holds for the irregular particles (Figure 4a, and b): the A/V ratio increases by 1.5 times from 4.85 to 7.28 cm⁻¹ and L decreases by 1.5 times from 2.25 to 1.50 cm; (iii) Therefore, the A/V×L values remain the same for each morphology regardless of the sizes, i.e., 10.92 and 6.0; (iv) The A/V×L for any sphere is invariantly 6, thus the minimum possible value of M is clearly 1. The example in Figure 4 demonstrates the M value increases with more irregularity, and this study witnesses the maximum value of M is about 3 for typical mineral particles based on the Krumbein and Sloss chart, which will be further discussed in Section 4.
Therefore, the proposed formula robustly explains the interrelation of M-A-V-L. The examples in Figure 1 can be now systematically described by the formula, $M = \frac{A}{V} \times \frac{L}{6}$, regarding how the other three parameters may change when one of the parameters is kept constant. In particular, the formula explains the ‘unilateral’ relation between morphology and size, i.e., the change of the particle morphology may change the size (Figure 1a), but the change of the particle size does not change the morphology (Figure 1c). It is clear that change of M impacts A, V, and L from the formula. On the other hand, the $A/V$ ratio is linearly proportional to $1/L$ for a given morphology, so the change of L is cancelled out by the change of $A/V$, which makes M invariant of the size, from which the ‘unilateral’ relation can be explained.

3 DESCRIPTION OF DISTRIBUTIONS OF INTERRELATED 3D PARTICLE GEOMETRY PARAMETERS

The proposed formula, $M = \frac{A}{V} \times \frac{L}{6}$, can be leveraged to graphically describe the distributions of interrelated 3D particle geometry parameters. Two different particle groups are numerically generated to demonstrate the efficacy of the proposed approach using the formula: (i) Mixed morphology group, where a total of 100 polyhedral particles are modeled with a variety of morphology such that the evaluated M ranges between 1 and 3. In Figure 5, the modeled particles are presented with the computed Sphericity, Roundness, and M. The particle size ranges from 3 mm to 9 mm. The sizes are deliberately controlled such that smaller particles tend to have a more irregular morphology. Therefore, this group is designed to have a clear relation between size and morphology; (ii) Near-sphere group, where another 100 polyhedral particles are modeled to be near-spherical. The modeled particles are shown in Figure 6, for which the Sphericity, Roundness, and M also are evaluated. The sizes are randomly selected between 3 mm and 9 mm. However, the particle shapes in this group are all similar to one another, so the evaluated M is near-uniformly distributed and close to 1. A 2D image of each particle is used to analyze the Sphericity and Roundness, for which the orientation with the maximum 2D projection area is selected as it is the most possible orientation when the particle is placed on a flat surface due to the higher stability (Bagheri et al., 2015). A Sphericity and Roundness analysis code by Zheng & Hryciw (2015, 2017) is adopted for the 2D image-based morphology analysis. A sample particle selected to demonstrate the interrelated geometry parameters is shown in the green circle in Figure 5, whose corresponding data points are marked in Figure 7. The size of the sample particle is 5.88 mm, and the computed Regularity $\rho$ (i.e., average of 2D Sphericity and Roundness) is 0.3955 (thus $1/\rho$ is 2.528).
Figure 5. Particle models of mixed morphology group evaluated with Sphericity, Roundness, and proposed M values. The particle in the green circle is selected as a sample particle for the demonstration of interrelated geometry parameters (See Figure 7).
Figure 6. Particle models of near-sphere group evaluated with Sphericity, Roundness, and proposed M values.
Figure 7. Description of the distributions of the ‘interrelated’ particle geometry parameters, where the parameter values of the sample particle (selected in Figure 5) are marked with green circle symbols; (a) Morphology distribution using conventional Sphericity and Roundness; (b) Particle size distributions for mixed morphology and near-sphere groups evaluated in terms of particle number and volume, respectively; (c) Combined description of M (= A/V×L/6) and size L compared to the description using the inverse of Regularity 1/ρ and size L. The M and 1/ρ of the selected sample particle are indicated in green; (d) Combined description of A/V ratio and V, which approximately follows a power law. The plots in Figure 7c and d are related using A/V = M/L×6, i.e., the A/V value in Figure 7d can be obtained from the corresponding data point in Figure 7c by dividing M by L. The volume V of the sample particle then can be found in Figure 7d, from which the surface area A can be also estimated by A/V×V; (e) Distributions of A/V ratio evaluated in terms of particle number and volume, respectively; (f) Distributions of M by volume.

The evaluated Sphericity and Roundness are plotted in Figure 7a. The data points for the mixed morphology group are spread over the space due to the variety of morphology, while those of the near-sphere group are concentrated in the upper-right corner due to the overall narrow range of morphology values with near-equidimensional and round shapes. Figure 7b shows the particle size distributions of the two groups that are evaluated by both the number and volume of particles and shown in terms of the cumulative percentage. The size distributions by the number of particles are practically same. However, the difference is more evident in the distributions evaluated by the volume, because the near-sphere particle has a higher volume compared to the irregularly shaped particle of the same size in the other group. This can be supported by the similar example in Figure
4, where the volume of sphere in Figure 4c is higher compared to the irregularly shaped particle of the same size in Figure 4b.

The interrelated distributions can be effectively described by leveraging two plots: (a) a plot showing the M distribution with respect to L (Figure 7c). This plot can also relate M and L to A/V, because $A/V = M/L \times 6$; (b) a plot representing the combined A/V ratio and V distribution that relates A/V to V (Figure 7d). The surface area A can be also estimated by multiplying x-axis value (A/V) by y-axis value (V). The interrelated distributions of M-A-V-L is thereby graphically preserved in these two plots.

The combined morphology M and size L distributions are shown in Figure 7c for both mixed morphology and near-sphere groups. The morphology is evaluated by both M and Regularity $\rho$. The inverse of Regularity ($1/\rho$) is plotted for consistent comparison against M because a higher $\rho$ represents near-equidimensional and round shape, while a higher M represents the opposite shape. This combined plotting clearly reveals the relation between morphology and size in the mixed morphology group as designated, i.e., the smaller the size is, the more irregular the morphology is. A similar trend is captured from both plots characterized by M and $1/\rho$. Figure 7c is a way that can combine the information from Figure 7a and b which are conventional plotting methods that characterize particle morphology and size separately. Figure 7c leverages a single plot with introduction to a new index M, where the valuable interrelation between the morphology and size is preserved unlike Figure 7a and b. Despite the similar trend for both plots using M and $1/\rho$, there is more data point scatter in the $1/\rho$ plot. This scatter is possibly due to (i) the uncertainty in selecting the single 2D projection plane, (ii) the inaccuracy associated with the 2D characterization of 3D particle morphology, and (iii) the characteristic of the reciprocal function $1/\rho$, i.e., $1/\rho$ significantly increases as $\rho$ gets smaller for low Sphericity and low Roundness as $1/\rho$ is a nonlinear curve. This characteristic may contribute to the seemingly more scattered data. Figure 7c also depicts the overall similar particle morphology distributions on the near-sphere group with M~1 and $1/\rho$~1, i.e., close to the minimum possible value for both descriptors. The plots shown in Figure 7c may be represented by 3D density distributions by leveraging the Z-axis as indicating the probabilistic density of samples with respect to M (or $1/\rho$) and L.

The combined A/V ratio and V distributions are shown in Figure 7d for both mixed morphology and near-sphere groups. The data points in Figure 7c can be related to the corresponding A/V ratio in Figure 7d as $A/V = M/L \times 6$. For example, the A/V ratio of the sample particle can be computed from Figure 7c, which is 1.886 mm$^{-1}$ ($= M/L \times 6 = 1.848/5.88 \times 6$). The volume V of the sample...
particle then can be found in Figure 7d, which is 32.13 mm$^3$. The surface area A can be also estimated by $A/V \times V$, which is 60.6 mm$^2$ (=1.886 mm$^{-1}$×32.13 mm$^3$). Therefore, the valuable information regarding the interrelation of M-A-V-L is graphically preserved in these plots. The conventional Regularity, however, cannot be used to describe the interrelation of the particle morphology to the other geometry parameters. Interestingly, the A/V and V in Figure 7d show a linear relation in log-log scale, i.e., follows a power law. The relation of A/V and V for the mixed morphology group can be approximated to $V = (A/V)^{2.64} \times 129.66$, and then to $\log(V) = -2.64 \times \log(A/V) + \log(129.66)$. The fitted line is shown with a slope of -2.64 in the figure. Considering the power value is -3 for sphere, i.e., $V = (A/V)^3 \times 36\pi$, the deviation is an interesting measure of morphology for the given group of the particles. The fitted line equation can be further simplified to $\log(V) = 1.61 \times \log(A) - 1.29$, which directly relates A with V. Using $A/V = M/L \times 6$, the power function can be also formulated to $\log(V) = -2.64 \times \log(M) + 2.64 \times \log(L) + 0.06$, which relates M, L, and V. The data for the near-sphere group can be also fitted to $V = (A/V)^{2.99} \times 116.26$, and similarly reformulated to find the set of relations. If the particles are perfect spheres, the relation can be analytically derived by $V = A^{1.5} / 6\sqrt{\pi}$. Therefore, the deviation of the power value may be used as a measure of morphology for the given group of the particles. Further investigation of the implication of the power value related to the morphology distribution is beyond the scope of this study and is left for future study.

The A/V distributions are evaluated by both the number and volume of particles and plotted in terms of the cumulative percentage in Figure 7e. The sample particle’s corresponding cumulative percentages are demonstrated in green in Figure 7e. Both plots by the number and volume of the particles depict that the near-sphere group maintains a higher cumulative percentage given an A/V ratio, in other words, a lower A/V ratio given a cumulative percentage. This is because the particle morphology in the near-sphere group is near-equidimensional and round, which makes the A/V ratio smaller, so the A/V plots are located on the left of those of mixed morphology group. Compared to the cumulative percentages by the number, the difference in the plots by the volume is much smaller, because the small particles in the mixed morphology group have a higher irregularity thus a higher A/V, while the large particles in both groups have overall similar morphology. Therefore, Figure 7e shows the cumulative percentages by the volume are similar up to 60%. This is supported by Figure 7f, where the M distributions are shown in terms of cumulative percentage by the volume. As shown in Figure 7f, the M distributions between the two groups are overall comparable up to 60%, meaning 60% of particles by volume have a similar morphology.
4 EXPERIMENTAL DEMONSTRATION OF PREDICTIVE CAPABILITY

4.1 Specimen Preparation for Laboratory Direct Shear Test

An experimental study is performed to demonstrate the predictive capability of the proposed formula to estimate the influence of particle geometry. A set of 3D particle models are developed and 3D printed for use in the direct shear test instead of using mineral particles to explicitly control the geometry parameters. The Krumbein and Sloss chart (Figure 8a) is referenced as the particle image library that is evaluated in terms of Sphericity and Roundness. The far different four morphology at the corners in the chart, i.e., 1-1, 1-5, 4-1, and 4-5, are selected. The Fourier descriptor-based modeling technique is used to generate a realistic 3D particle model from the 2D cross-sectional images (Mollon and Zhao, 2013). The developed 3D models are shown in Figure 8b with the evaluated M for the models. The particle 4-1 is the most irregular among the four morphology and therefore has the highest M value of 2.71. The irregularity evaluated by M (3D descriptor) is in order of 4-1 > 4-5 > 1-1 > 1-5 (i.e., M = 2.71 > 1.96 > 1.36 > 1.08). Regularity ρ (2D descriptor) is also evaluated, and 1/ρ is shown in the figure. The irregularity evaluated by 1/ρ is in order of 4-1 > 1-1 > 4-5 > 1-5. Both M and 1/ρ estimates the particle 4-1 is the most irregular, and 1-5 is the opposite. However, the order of 1-1 and 4-5 is different. It appears that 1/ρ estimates the contribution of particle 1-1’s angularity (intermediate scale) is higher than the particle 4-5’s elongation (global scale). The Krumbein and Sloss chart represents the morphology of typical mineral particles. Therefore, it is anticipated that the upper bound of M value for the typical mineral particles is about 3, which indicates a highly irregular morphology that can be found in nature.

![Figure 8](image-url)  
Figure 8. Development of 3D particle models and 3D printed particles; (a) Representative 2D morphology of typical mineral particles evaluated in terms of Sphericity and Roundness, modified from Krumbein and Sloss (1951). Particles are numbered in ‘row # – column #’ format for convenience; (b) Developed 3D particle models and the morphology quantified using $M = A/V \times L/6$, and the inverse of Regularity, $1/\rho$; (c) 3D printed particles of the four models; (d) Direct shear test setup.
The developed 3D particle models are then 3D printed (Figure 8c) for laboratory direct shear test (Figure 8d). Form 1+ Stereolithography (SLA) printer is used for the 3D printing (Formlabs, 2014). Particles are printed in 25 microns of layer thickness. Therefore, the surface texture of printed particles is controlled as the particles are printed using the same material at the same printing resolution. The compressive strength and the elastic modulus of the printed objects are roughly comparable to those of Florida limestone (Su et al., 2017). The cylindrical shear box size is 63.5 mm (2.5 in) in diameter × 37 mm (1.5 in) high. The each particle model is scaled to have the same volume (11.67 mm$^3$) such that a same number of particles can be considered per test specimen.

The combined descriptions of the morphology and size are evaluated in terms of $M$ and $L$ as shown in Figure 9a, and the evaluated $1/\rho$ are also plotted for comparison. The four particle models are controlled to have the same volume of 11.67 mm$^3$, and therefore, it is obvious that the particle size increases with the morphological elongation and angularity as the size is measured in terms of the bounding sphere diameter. Consequently, the near-spherical particle 1-5 is the smallest as 3.05 mm, while the most irregular particle 4-1 is the largest as 5.97 mm. This trend is reflected well with $M$ and $L$ in Figure 9a, which increase together in order of 1-5, 1-1, 4-5, and 4-1. A similar tendency is shown for $1/\rho$ and $L$ except the particle 4-5 that is out of the trend, i.e., $1/\rho$ decreases while $L$ increases. Figure 9b depicts the combined description of $A/V$ and $V$, where the same trend is observed in order of 4-1 > 4-5 > 1-1 > 1-5 from the largest $A/V$. The same order is also estimated for the surface area $A$ because all particles have the same $V$. Considering the evaluated $M$ and the interrelated geometry parameters, the same trend of the mechanical performance is anticipated from the laboratory testing in order of 4-1 > 4-5 > 1-1 > 1-5. Each specimen is uniformly graded in terms of morphology and size, i.e., composed of identical particles of same morphology and size. Therefore, the evaluated $A/V$ distributions are shown as vertical lines as plotted in Figure 9c.

The adopted particles are relatively large compared to the mineral particles typically used in the direct shear test, because it is challenging to 3D-print smaller particles due to the extensive labor work necessary to post-process a larger number of particles, and also due to the limitation of the smallest possible layer thickness to represent details of the particle shape. However, the adopted sizes conform to the requirement of ASTM D3080/D3080M (2011).

The four specimens of particles 1-1, 1-5, 4-1, and 4-5 are controlled to have the initial void ratio of about 0.73. The specimens are tested at four different normal stresses, 40.5, 102.5, 164.4, and 226.4 kPa. The rate of shear is maintained at 1 mm/min.
4.2 Test Result and Discussion

Each test is repeated three times, from which average response is obtained. No particle breakage or significant particle deformation is observed at the end of tests. Figure 10a-h show the average responses of shear stress and vertical displacement at the four different normal stresses. While limited stick-slip fluctuation is shown in the test, the observed mechanical behavior is overall consistent in order of 4-1 > 4-5 > 1-1 > 1-5 from the highest to the lowest shear strength and modulus as shown in Figure 10a-d. The friction angles evaluated from the shear stress responses are shown in Figure 11, which clearly shows the strengths in the order. A similar trend is shown for the vertical displacement in Figure 10e-h with the specimen of 4-1 showing the highest rate of dilation. The nature of vertical displacement of 4-1 is also different from the other specimens, i.e., the vertical displacement of 4-1 shows an overall continuous increase until the end of the test, while the responses of other specimens are flattened out. The difference is possibly attributed to the different relative densities of the specimens affected by the particle morphology. A higher range of void ratio is typically obtained with higher particle irregularity as broadly evidenced in works of literature (Cho, Dodds and Santamarina, 2006; Abbireddy and Clayton, 2010; Maeda et al., 2010). Despite the initial void ratio in all specimens controlled to 0.73, it is observed the relative density (evaluated based on the maximum and minimum void ratios) of specimen 4-1 is about 85% (i.e. relatively very dense), while those of the other specimens are less than 25% (i.e., relatively loose). Therefore, the specimen 4-1 is able to continuously dilate while being sheared. The difference in vertical displacements of the specimens 4-5, 1-1, and 1-5 is relatively unclear with limited stick-slip fluctuations due to the large particle sizes adopted in the test. The fluctuation in the response
clearly occurs when the contact network in the granular system is re-organized under a given loading condition. The shear box contains a limited number of particles due to the relatively large particle size, there is a limitation in sensitively representing the vertical displacement. Notwithstanding the fluctuation, a trend of a higher rate of dilation rate is shown for 4-5 compared to 1-1 and 1-5.

The test result demonstrates that the proposed approach can reasonably relate the particle scale information to the macroscopic mechanical property by its order and corroborates its predictive capability to estimate the influence of particle geometry. Furthermore, all the particles used in this study pass through 4 mm sieve and are retained in 2 mm sieve. Therefore, these specimens are equally classified as uniformly graded sands according to the conventional Unified Soil Classification System despite the significant differences shown in the test results. This research finding indicates the current specification remains to be improved for enhanced soil classification.

5 CONCLUDING REMARKS

This study proposes a new formula, \( M = \frac{A}{V} \times \frac{L}{6} \), that interprets the 3D particle morphology \( M \) in terms of the other particle geometry parameters, i.e., surface area \( A \), volume \( V \), and size \( L \). Therefore, this ‘marvelously’ simple formula enables to clearly unravel the interrelation of \( M-A-V-L \), and allows for the systematic understanding of the particle geometry effect. The new formula can be leveraged to robustly describe the distributions of the interrelated 3D particle geometry parameters. Therefore, the proposed approach will help quantitatively relate the particle scale geometric information to the macroscopic property of granular materials, and significantly enhance the predictive capabilities. A challenge of applying the proposed approach to the engineering practice may be concerned with measuring the surface area of mineral grains. This measurement can be obtained by using optical characterization techniques such as photogrammetry. Notwithstanding such techniques are computationally expensive at the moment, the proposed approach is sustainable in the sense that the 3D object scanning becomes more accessible and affordable with newer generations of imaging equipment and the advances in the image processing algorithms in the future.
Figure 10. Direct shear test result: stress-strain curves and vertical displacements obtained at four different normal stresses (40.5, 102.5, 164.4, and 226.4 kPa); where the stress-strain curve in (a) to (d) is normalized by $\tau_{\text{max}}^*$, maximum shear stress obtained from the specimen 4-1.
Figure 11. Friction angles evaluated from the fitting lines of shear strengths.

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