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Applying 2D shape analysis techniques to granular materials with 3D particle geometries

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Abstract. It is well established that particle geometry is a key parameter influencing the response of a granular material as well as its packing density. There are many challenges associated with obtaining data for full 3D quantification of the geometry (shape) of large numbers of particles. Consequently we typically assess particle shape by considering two dimensional images of the particles. This paper proposes a technique for developing a three dimensional description of particle geometry by combining sets of two dimensional images with multiple orientations. The paper establishes a relationship between the two-dimensional measure of particle geometry circularity (as defined by ISO standard 9276-6 / 2006) and the three-dimensional measure sphericity as defined by Wadell. An analytical comparison between these measures is achieved by considering a set of scalene ellipsoids (with three differing principal diameters). Each ellipsoid was systematically rotated to obtain a set of 2D projections and the circularity of each projection was quantified. The results indicate that there is a close relationship between the mean circularity and Wadell's sphericity. The results of this analysis have implications for modern image analysis based technologies that can automatically assess the shape of large numbers of particles. Data for real coarse sand size particles obtained using the QicPic apparatus (Sympatec) are reviewed in light of the findings of the analytical parametric analysis.

Keywords: Shape analysis, scalene ellipsoid, sphericity, circularity.

PACS: 01.30.Cc, 81.05.Rm

BACKGROUND

Quantifying particle shape is the most basic characterization of a granular material, whether considering natural granular materials such as soil or food grains or processed granular materials such as detergent powders or pharmaceutical tablets. The objective of this paper is to highlight the challenges associated with using 2D metrics to characterize the shape of 3D particles. When quantifying particle shape the most basic description made is quantification of the particle form (e.g. how spherical the particle is). We can refine our scale and consider angularity and roughness; however these characteristics are outside the scope of the current study. While various methods to quantify particle geometry have been proposed since the beginning of the twentieth century, their use was rather academic as obtaining and analyzing accurate measurements of statistically representative numbers of particles was intractable. Instead engineers and scientists tended to quantify shape by a comparison of a (limited) number of particles with a standard reference chart, e.g. the reference charts proposed by Powers [1] or Krumbein and Sloss [2]. In

recent years due to the advent of digital cameras and image analysis algorithms, we can more easily access and analyze 2D images of large numbers of particles. However, these methods are limited as we are quantifying the geometry of three dimensional bodies using two dimensional projections of their form. This paper discusses the implications of this limitation, using theoretical analysis of smooth convex particles and detailed measurements of artificial, angular particles in the range of coarse sand.

CIRCULARITY VERSUS SPHERICITY

Typically particle form is quantified using either sphericity or circularity, i.e. how close is the particle geometry or 2D projection to a perfect sphere or circle respectively. A number of definitions of circularity and sphericity have been proposed in the literature and some of these are presented in Table 1. While SA_{es} is the surface area of the sphere with the same volume as the particle, SA_{rp} is the real surface area of the particle. A and P are the area and the perimeter of any horizontal projected section Λ of the particle at rest;

TABLE 1. Definitions of sphericity and circularity

Reference		Symbol	Expression
Wadell (1932) , (1935)	[3] [5]	degree of true sphericity, ψ	$(SA_{es})/(SA_{rp})$
Wadell (1933)	[4]	degree of sphericity, ϕ	$2\sqrt{A/\pi}/d_{cmin}$
ISO (2006)	[6]	circularity, C	$4\pi A/P^2$
Krumbein and Sloss (1963)	[2]	sphericity, S_{KS}	“related to the proportion between length and breadth of the image”
Cho et al. (2006)	[7]	sphericity, S_{CE}	d_{imax}/d_{cmin}
Sympatec (2007)	[8]	sphericity, S_Q	$2\sqrt{\pi A}/P$

d_{cmin} and d_{imax} are the perimeters of the minimum circumscribed and the maximum inscribed circles to the section Λ . As one can see from Table 1, the parameter S_{KS} was not clearly defined [2]. Here the interpretation of S_{KS} presented by Cho et al. [7] is assumed (i.e. $S_{KS} = S_{CE}$). Note that the Sympatec [8] definition was proposed for use on binary images of particles obtained from taking photographs of particles falling under gravity using the QICPIC apparatus.

Method of evaluation

The applicability of the various sphericity and circularity descriptors to quantify particle form were firstly examined from a theoretical perspective by considering a scalene ellipsoid, a particle whose geometry can be analytically described as in Krumbein and Sloss [2]. A scalene ellipsoid is an ellipsoid that has three distinct principal diameter values given by d_1 , d_2 , and d_3 . The principal axes associated with these three diameters are named the major, intermediate and minor principal axes, respectively. A two dimensional schematic diagram of a scalene ellipsoid, considering a plane through its centroid, orthogonal to the minor principal axis is illustrated in Figure 1. The particle is rotated about its minor principal axis so that the inclination of the major principal axis to the vertical is given by α . If an image of the particle orthogonal to the current view was captured from a camera located above or below, the observed projected major diameter is denoted d_p .

For the elliptical two dimensional geometry illustrated in Figure 1, if we consider any diameter with length d , there exists a second “conjugate diameter” of length d_c so that $d^2 + d_c^2 = d_1^2 + d_2^2$. As indicated in Figure 1, the tangents at the interception of d_c with the ellipse surface will be parallel to the diameter d . We define β to be the minimum angle between the major principal axis and the conjugate to the vertical diameter. From knowledge of the geometrical properties of an ellipse,

the following relationships hold:

$$\begin{aligned}\beta &= \arctan[(d_1/d_2)^2 \tan \alpha] \\ d_c &= [(d_1 d_2)^2 / (d_2^2 \cos^2 \beta + d_1^2 \sin^2 \beta)]^{0.5} \\ d_p &= d_c \sin(\alpha + \beta).\end{aligned}$$

There is no exact expression for the perimeter of an ellipse, required to calculate the parameters C and S_Q . For this study, the values of P were calculated using the approximate formula proposed by Hudson [9].

As noted above, Wadell’s “true sphericity” Ψ can be calculated by considering the ratio of the surface area of the sphere whose volume equals the ellipsoid volume and the actual surface area of the ellipsoid. For a scalene ellipsoid, an exact closed form solution for the surface area remains undefined. However, in agreement with Kingston et al. [10], it has been accepted that the equation proposed by Thomsen [11], gives a good approximation and it is adopted here.

To compare analytically the relationship between circularity measurements of two dimensional projected

FIGURE 1. Conjugate diameters and normal projection of an ellipse giving a dimension d_p .

images and the real three dimensional geometry, a number of scalene ellipsoids were analysed in detail. In the study 15 combinations of d_1 , d_2 , d_3 were considered. The range of ellipsoids analysed can be appreciated by reference to the Zingg [12] diagram, presented in Figure 2. The Zingg diagram is a simple graphical approach to characterize form that recognizes the 3D nature of particle geometry. In the Zingg diagram the particle form is described by plotting the ratio of the intermediate and major principal diameters (d_2/d_1) along the y axis and the ratio of the minor and intermediate diameters (d_3/d_2) along the x-axis.

FIGURE 2. Aspect ratio of the considered ellipsoids in Zingg's diagram ($d_1 > d_2 > d_3$).

Each ellipsoid considered was rotated around each of its principal axes $n=10$ times. For each series of rotations around a given axis, the inclination, α , illustrated in Figure 1, was varied in the range 0 to $\pi/2$ in increments of $\pi/20$. Therefore, for each ellipsoid, 33 ellipses were projected onto the projection plane (Figure 1). This approach yielded a total of 495 ellipses for analysis.

For each ellipse considered the circularity C_{ij} was calculated. The subscript j indicates the axis the parent ellipsoid was rotated about to generate the ellipse (1=major, 2=intermediate, 3=minor). The subscript i indicates the value for α ($\alpha=i\pi/20$). Then, for each ellipsoid a value of mean circularity, C_{mean} , was calculated as:

$$C_{\text{mean}} = \frac{1}{3(n+1)} \sum_{i=0}^n \sum_{j=1}^3 C_{ij} \quad (1)$$

Figure 3 considers the variation of both C_{mean} and Ψ with the elongation ratio d_2/d_1 . The d_2/d_1 values vary in the range 1/3-1, giving a series of curves for Ψ and C_{mean} for three different flatness ratios $d_3/d_2=1/3$, 2/3 and 1. The curve C_{12} , representing the circularity of the principal section (112) is also illustrated in Figure 3.

The values of Ψ and C_{mean} are less sensitive to the particle elongation (d_2/d_1) than C_{12} . The differences between the values of Ψ , C_{mean} and C_{12} are within 10% when $d_2/d_1 \geq 0.5$ and when $d_3/d_2 \geq 2/3$. For the flattest particles considered ($d_3/d_2=1/3$), the curves for C_{mean} and Ψ are furthest from the curve C_{12} . The difference between C_{mean} and Ψ is less marked as the elongation approaches 1 if the flatness ratio is $\geq 2/3$. For the flattest particles a different trend is observed with close agreement between Ψ and C_{mean} , their values being equal for $d_2/d_1 \approx 0.45$.

FIGURE 3. Sensitivity of different sphericity parameters for the set of considered ellipsoids.

This analytical study confirms our intuitive understanding that the appropriateness of using measures of form derived from 2D images decreases as flatness increases and the contribution of this study is to enable the limitation to be quantified. Measurement of circularity even in 2D requires the use of image analysis. Measurements of elongation can more easily be made, and Figure 3 allows also the values of C_{12} to be interpreted in terms of elongation.

FIGURE 4. Cross-section of crushed pasta (linguine), captured by AxioSkopec40 optical microscope.

The applicability of the findings of this analytical exercise to real particles with more angular geometries and in the size range of a coarse sand was considered by looking at particles made from crushed pasta (linguine) with elliptical cross-sections as illustrated in Figure 4. Following crushing, the particles were sieved so that only particles in the size range 1.18 mm to 2.00 mm were examined. Detailed measurements of 9 representative particles were made. These detailed measurements were achieved using optical microscopy (AxioSkope40) and image analysis [13]. The area and perimeter of the particle in the 112 plane were measured (orthogonal to the minor principal axis), as well as d_1 , d_2 , $d_{\min}$, $d_{\max}$. A particle was rotated vertically by 90° , and using small lateral supports, the particle area, perimeter, and measurements of d_2 and d_3 in the 213 plane (orthogonal to the major principal axis) were obtained; d_2 and d_3 values of other particles were checked using a digital micrometer and were found to be very repeatable with a standard deviation of about 1%.

The measured data were used to calculate ψ , S_{KS12} , S_{KSmean} , C_{12} , S_Q , C_{mean} . S_{KSmean} and S_Q values were calculated as the arithmetic mean of the values for particle views in the 112, 213, and 311 planes. Figure 5 presents the variation in each of these parameters with the calculated values for ψ . As can be observed from Figure 5 the S_Q values provide the best approximation to the true sphericity (ψ) values, as the S_Q consistently overestimate the true sphericity values but by less than 0.10. The C_{12} values are also relatively close to the ψ values but the trend is not consistent, and sometimes $C_{12} < \psi$, sometimes $C_{12} > \psi$. The C_{mean} values are consistently less than ψ and their divergence is slightly greater than for the S_Q values, being up to 0.12. Neither the parameter S_{KS12} nor the parameter S_{KSmean} gives a good approximation to ψ .

FIGURE 5. Scatter of several form parameters versus Ψ .

It is interesting to note that the C_{mean} values are less representative of the ψ values than C_{12} , suggesting that there is some merit in Wadell's observation [5] that the 2D images he described by ϕ (Table 1) often sufficed for 3D characterization of particle sphericity.

The particles selected for detailed analysis were representative of a statistically significant number of particles. In a QICPIC test involving 620 images, the S_Q values were observed to range between 0.71 and 0.87, with 50% of the particles having an S_Q smaller than 0.85. In the detailed study the sphericity values ranged from 0.84 to 0.90, with 5 out of 9 particles having an S_Q less than or equal to 0.87.

CONCLUSIONS

For very flat particles, such as scalene ellipsoids with a small ratio of d_3/d_2 (0 to 0.6), 3D measurements are essential to capture the particle form. However when the flatness is less pronounced, e.g. scalene ellipsoids with a large ratio of d_3/d_2 (0.6 to 1), a good approximation of 3D form can be achieved using 2D images. On the other hand, in the case of blade-like particles, i.e. the very elongated scalene ellipsoids, with a small ratio d_2/d_1 ($<1/3$) and very flat ($d_3/d_2 < 1/3$), 2D images are again representative of 3D sphericity.

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