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Determination of minimum pixel resolution for shape analysis: Proposal of a new data validation method for computerized images

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ABSTRACT

In many different research areas not only size, but also an exact description of particle shape is important in order to understand certain physical or chemical processes. Digital image analyses with specially developed software (DIP) have become increasingly popular in recent years, producing a huge amount of reproducible data. However, since image captures are pixelated, purely digitalisation problems/errors may occur and, hence, a minimum number of pixels for meaningful results has to be established. This may depend on different computer software or on calculation methods. Here we bring *Elongation*, *Circularity* and *Sphericity* in relation and calculate in a theoretical model maximum values of *Circularity* and *Sphericity* for specific *Elongation* values from 0 to 1. In these simple 2-dimensional plots, which can be applied to any DIP program, a line marking the upper limit of congruent shape analysis can be calculated. Points that fall far above the theoretical maximum curve are interpreted as digitalisation issues of the DIP programs: especially measuring the boundary length (perimeter) is not as simple. It can be shown that, with increasing particle size, the rate of obvious erroneous shape analysis data decreases, and thus a minimum pixel number can be established after “pixel size cleaning”. We tested our model with two commonly used plugins with two different shape calculation methods for particle analysis of the DIP program *ImageJ*: while an object has to be build-up of about 200 pixels using the preinstalled plugin, the threshold can be significantly reduced (50) using the *Particles8_Plus* plugin by *Landini.*

1. Introduction

The characterization of particles is important in different research areas like Geology, Biology, Pharmaceutical Sciences, Agricultural and Biological Sciences, Materials Science etc. Traditionally, grain size and shape analysis have been the object of study for Sedimentologists because many Palaeoclimate and Geology aspects of the source area, transportation processes, depositional processes and diagenetic processes of sedimentary rocks can be inferred from the morphological characterization of these petrological materials [1]. Moreover, size and shape define the geometric arrangement of particles (packing). Thus, porosity, fluid interactions or physical resistance can be deduced, which is of much interest in Engineering Geology in order to understand, for instance, soil behavior. Pharmaceutical technology filling, especially the coating of pellets, depends on a detailed characterization of the morphology of particles [2] so that their analysis becomes increasingly interesting as it extends the scope of application to the food engineering field [3–7]. In the industrial environment sector, the study of morphology parameters of fillers play an important role in different application areas like chemical or construction industries (paints, cosmetics, mortar, concrete, ceramics, etc.). Early on in the 20th century, the light microscope was successfully employed to determine average the particle size and particle size distribution of the filtration clays or minerals used as pigments and fillers, and also of other very finely divided substances [8–10]. Furthermore, the importance of both size and shape for the total surface characterization of a specific particulated material was acknowledged [11].

While grain (particle) size distribution has been established for a wide range of applications, e.g., the Udden-Wentworth scale [12], or more specifically in particular fields like Fine Arts [13], shape has often been disregarded. This is probably due to the difficulty of providing an accurate estimate, and given the time-consuming measurements and calculations that its characterization involves. In line with this, it is worth mentioning that the advances made in computer sciences over the last two decades have significantly improved the results obtained by digital image analysis/processing (DIP). The benefits of using computer technology are obvious: a large number of measurements can be taken in a short time, and they provide an economic, consistent and objective analytical method.

In turn, some technical difficulties appear when incorporating computational technologies into stereological studies, such as the additional step of the conversion of RGB, CMYK, 8-bit Grayscale images, etc. into a Binary Image (thresholded), which most image processing programs need. In addition, the latter can result in the loss or distortion of the information contained in the original image. Moreover as any digital image is a build-up of pixels, a minimum number of pixels has to be fixed for the proper description of the feature under study,

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at least when carrying out a shape analysis. This lower limit can differ for each shape parameter, so it would be interesting to develop an experimental protocol to establish the level of accuracy obtained when an image processing program is applied to a feature defined by a specific group of pixels.

This paper reports the preliminary results obtained in a research project which aimed to study the morphological characterization of particulated materials. This can be done by three dimensional methods (e.g., [13–15]) or by two dimensional or projection methods. This paper addresses only projection methods because they must be employed for examinations by light microscopes. This novel method enables the determination of the minimum pixel resolution of a particle in a digital image to accomplish a particular level of accuracy in the determination.

This method has been implemented on the pigments used in Fine Arts during different historical periods to provide a reliable estimate of the size and shape of these artists' pigments. Nevertheless, the proposed method can also be applied to other research and industrial fields which deal with the micromorphological characterization of particulated materials. In the specific Fine Art and Conservation of Cultural Heritage field, these morphological data can prove useful to comprehend the dispersion processes of pigments in paint layers [16] or to provide useful information to supplement information on the chemical composition for provenance studies in works of art provided by other instrumental techniques [17].

2. Theoretical Model

2.1. Theoretical Parameters for Shape Description

There are many different ways to characterize a particle in two or three dimension, either geometrically/mathematically or by a visual comparison chart [11,12,18–27]. The most common definitions used for particle shape description are listed below:

The *Circularity (C)* of Cox [23] defines the deviations of the shape of a particle from the circular shape. It uses the *Area (A)* and the *Perimeter (P)* ratio of the particle:

$$C = \frac{4\pi A}{P^2} \tag{1}$$

Although the term '*sphere*' refers to a perfectly round geometrical object in three dimensions, '*Sphericity*' can be used to describe objects in two dimensions. Riley [25] proposed the inscribed circle *Sphericity* (φ), which is defined as the square root of the ratio of the inscribed (D_i) and circumscribed circles (D_c):

$$\varphi = \sqrt{\frac{D_i}{D_C}} \tag{2}$$

While the first two shape descriptors are sensitive to particle roundness, the *Convexity Ratio* and *Solidity* are sensitive to the surface roughness of a particle. The *Convexity Ratio (CR)* can be calculated by dividing the *Convex Perimeter (hull, Convex_hull)* by *Perimeter (P)* and *Solidity (S)* by dividing *Area (A)* by the *convex area* (*Convex_A*). *Perimeter* (*P*) follows the exact contours of the particles, while the *Convex Perimeter* (*Convex_hull*) is like a rubber band. The *Convex Area* (*Convex_A*) is the area enclosed by the *Convex Perimeter*. [22].

$$CR = \frac{Convex\_hull}{P} \tag{3}$$

$$S = \frac{A}{[Convex\_A]} \tag{4}$$

These parameters have been well-established and are frequently used to describe particles.

Another commonly used parameter is the *Aspect Ratio (AR)*. This shape description factor combines the measurement of two axes and is an indicator of particle elongation. Nevertheless, it is still ambiguous as to which dimension should be measured (e.g., axes of best fit ellipses, maximal Feret, minimal Feret, Feret 90º to maximal Feret, dimensions of minimal bounding rectangle/box) and whether the longer dimension should be divided by the shorter one, or the inverse [3,28–33]. Commonly, length is divided by breath and results in values of *AR* ≥ *1*, but once again, there is often no mention of which dimensions are measured. However, this is very important to calculate three shape factors: *Roundness*, *AR* and *Elongation*.

Some authors [3,29,33] used *Reciprocal AR* (*1*/*AR*) as an *Elongation (E)* value, but here we propose the elongation calculation as follows:

$$\mathrm{E} = 1 - \frac{1}{\mathrm{AR}} \tag{5}$$

While *AR* values range from 1 to infinite, the objective of both calculation methods, *Reciprocal AR* and *Elongation*, is to provide a result that falls in the 0 and 1 range (like other form factors: *Circularity, Roundness, Sphericity, Convexity Ratio and Solidity*).

Although this is only a scaling/definition problem, and not a different calculation method, we prefer this definition for the following reason:

In all common definitions, a circle takes a value of $AR = 1$ and *Circularity* = 1. Thus it follows that *Reciprocal AR* is also 1, unlike the definition above, as elongation would result in 0 (a circle is not elongated) and an extremely elongated particle would result in almost 1.

2.2. Relation Area/Perimeter for Different Particle Shapes and the Resulting Maximum Circularity and Sphericity Values for a Specific Elongation Value: Preliminary Considerations

In the previous section, common shape parameters, and irrespectively of each other, have been generally discussed. Here three shape parameters are elated to each other: *Circularity-Elongation* and *Circularity-Sphericity*. In Eq. (1), the dependency of the *Circularity* value of the Area and Perimeter can be seen. Eq. (2) also shows how *Sphericity* and *Elongation* are calculated. In order to find the maximum *Circularity* or *Sphericity* value for a specific *Elongation* value, some preliminary considerations have to be made.

The area of a regular polygon with n edges can be calculated by the following formula:

$$A = D_c^2 \sin\left(\frac{2\pi}{n}\right)\frac{n}{2} \tag{6}$$

and the perimeter is:

$$P = D_c 2n \sin\left(\frac{\pi}{n}\right) \tag{7}$$

where $D_c = \frac{a}{2\sin\left(\frac{\pi}{n}\right)}$ (circumscribed circle); inscribed circle $D_i = \frac{a}{2\tan\left(\frac{\pi}{n}\right)}$

For $n \to \infty$ (circle): $A = \pi r^2$, $P = 2\pi r$; $r = D_c = D_i$

From the above formulas, it can be seen that the A/P ratio, and thus *Circularity C*, increases with the number n of the regular polygon to reach the maximum value for a perfect circle (r/2, $C = 1$). Alternatively, i.e., for the same perimeter of a circle and a square, it follows that the area of the circle is 4/π ~ 1.27 times greater than the square. In a 2-dimensional plot, the same occurs for *Sphericity* φ: with n increasing the difference between the inscribed and circumscribed circle radii to become smaller, consequently φ increases ($\varphi = 1$ for a circle, $D_c = D_i$).

Elongation depends on the *Aspect Ratio* definition, as previously mentioned. Irregularly and jagged shaped particles (low *Solidity* and *Convex Ratio*) have a relatively large perimeter, thus *Circularity C* decreases for the same elongation values. The highest *Circularity C* for a specific low *Elongation E* value (close to 0) can, therefore, be found only in regularly shaped particles, like regular n-edge polygons,