

Quantitative measures for shape and size of particles

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Abstract

Previous efforts to define these terms are reviewed and their deficiencies noted. New quantitative measures of size and shape are proposed, based upon measurements made possible by image analysis techniques. These may be applied to both single particle and to assemblages of particles. Laboratory test results are presented to demonstrate the application of one of the new measures. Suggestions are made for further research. © 2002 Elsevier Science B.V. All rights reserved.

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1. Introduction

The importance of particulates ranges across many fields with large economic impacts. For example, in 1999, the construction industry of the USA used about 2.5 billion tons of rock products. At the other end of the mass scale, the pharmaceutical industry uses relatively small amounts of materials. However, each industry has an annual economic impact in the tens of billions of dollars. Some other fields in which the properties of end products are strongly influenced by the geometry of the particulates employed include materials science, food, soils, catalysis, pharmacology, and nanotechnology. Three of the most influential characteristics are shape, size, and surface texture. Owing to limitations of space, the present paper considers size and shape only; surface texture is treated elsewhere [12].

2. Geometry of individual particles: size and shape

Size and shape are the two terms most commonly encountered in describing particles. However, despite much work by many authors, to date, there is no generally accepted quantitative definition of shape (and still some difficulties with size as will be shown hereinafter).

2.1. Size

A typical scientific definition of size is: “the amount of space occupied”, or “the volume occupied”, or simply “the volume”. A regular body can be described as one with a shape defined by surfaces that are well defined mathematically. For such regular bodies, the volume can be calculated. For irregular bodies, size must be measured or estimated. The measurement technique known as displacement (first reported by Archimedes, and little improved upon since then) can be used to estimate the volume of a single particle or a sample containing a small number of particles. However, for very large number of particles (typical in the real world), this is not practical. Consequently, the most current “definition” of size in most fields is an operational one in which a standardized sample is shaken through a standardized set (“nest”) of sieves and the fractional weight of the sample retained on each sieve recorded. If the density of the particles is constant, then the mass, weight, and volume (but not necessarily number) distributions are the same. Operational definitions are published by ASTM or equivalent authorities: they have become popular for their ease and efficiency. However, any definition of size based upon sieves is not unambiguous as may be seen from Fig. 1. Such procedures are incapable of providing three-dimensional information.

2.2. Shape

Early and natural attempts to “define” shape compared the shape of a particle to that of some object of regular

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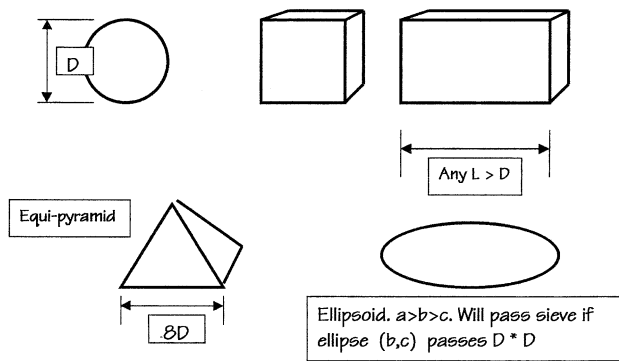


Fig. 1. Particles which meet the definition of “Size D” by any sieve procedure.

geometry (presumed to be well known to others). Popular reference shapes found in the literature and in anecdotal use include the sphere, cube, parallelepiped (also called cuboid, ashlar, or simply brick), ellipsoid, tetrahedron, and the five Platonic solids. It was soon recognized that such descriptions were only of qualitative use.

Alternative proposals then considered an “equivalent particle” which is defined by selecting two items, (a) a reference shape (e.g., cube or sphere) and (b) some selected features (e.g., surface area or volume). By equating the feature in the two particles, one may calculate the size of the “equivalent” reference shape. For example, if a real particle has surface area, S , and volume, V , one may select a reference shape (say the cube) and then select some property (say surface area) by which to construct the “equivalent” particle. In this example, the equivalent particle is termed the “equivalent surface area cube” (ESAC) and is simply the cube which has the same surface area as the original particle. In the given example, the ESAC has side dimension $= S/6$. The “equivalent volume cube” (EVC) would have sides of $(V)^{1/3}$, the “equivalent volume sphere” (EVS) would have diameter $(6V/\pi)^{1/3}$, etc.

With a wide range of regular shapes and properties from which to choose, it is possible to construct a large number of these indices. While such characteristics often serve as useful qualitative descriptors of particles and groups of particles, they have proven to be of limited value for quantitative purposes. A particular problem is that the numerical value of the “feature” (surface area volume, etc.) must be known: this information is not always available.

Yet another approach is to use the ratio of such geometrical quantities as an index of shape in the hope that some useful information can be obtained by comparing the value of this ratio with the value of the ratio for some regular solids. For example, the ratio of (volume/surface area) for a sphere of diameter D is $(D/6)$, which is, interestingly, the same for a cube. If one can obtain this ratio for a given irregular particle, it can be compared with the cube, sphere, etc.

These ideas, and many examples, are discussed exhaustively in the literature: e.g., Mather [5,6], Feda [3], and Russ [9–11].

3. Size and shape of real bodies

The vast majority of real particles do not have regular shapes; their properties cannot be calculated and must be estimated by some means. Since shape and size are purely geometrical properties, there are two ways in which they may be described. These are termed the boundary method and the assemblage method.

In the boundary method, the size of the body is defined as “the volume enclosed by its boundary” (the shape of the body is generally assumed to be the same as the shape of the boundary). If the boundary can be described numerically, analytical methods may be used to create a mathematical approximation to the surface. Examples in 2-D include Beddow [2] and, in 3-D, Garboczi and Martys (2001). As the power of computer increases, 3-D methods are now practical enough for industrial use.

In the assemblage of elements method, the entire body is replaced by a number of smaller, component elements. These may be of any size or shape (but these must be known). For convenience, assume these to be small cubes (or voxels) of unit side (and hence unit volume). These restrictions do not invalidate what follows.

The size of the body can then be regarded as the sum of the volumes of its component elements. If the volume of a voxel is taken either as unity or as the unit of measurement, then the volume is simply a dimensionless count, e.g., “This body occupies 13 unit volumes of space”.

The shape of a body may now be defined as “the spatial distribution of its component elements”. This is impossible to describe concisely: in fact, if sufficiently small voxels are used, every body will have a unique shape and size. However, the assemblage approach does suggest statistical measures of size and shape as described hereinafter.

These definitions have academic appeal but require methods for defining either the coordinates of points on the surface (boundary method) or the coordinates of points within the mass (assembly of elements) in order to be useful.

4. Discrete numerical modeling for size and shape using assemblage of elements (voxels) approach

As noted, the definitions offered above are useless unless the coordinates of many points (either on or in) a particle can be found. Recent developments in metrology make this possible, including,

- (a) digital (external) imaging,
- (b) surface profilometry,
- (c) tomography (reconstruction of internal features by invasive and non-invasive interrogation techniques).

Some of these methods (e.g., c) offer true three-dimensional approximations while (a) is necessarily restricted to two dimensions.

For (a), a typical technique is to photograph the body from many directions (producing shadowgraphs or silhouettes or projections) and to use measures from the photographs to characterize the geometry of the body.

In (b), a device performs an external scan of the body and produces an array of coordinates (x, y, z) , (relative to some known coordinate system) for points on the surface of the body. Techniques include laser ranging, acoustic ranging, direct mechanical probing, and speckle interferometry. The result is a three-dimensional array of coordinates of points on the surface. The user must then select a method for using these coordinates to estimate the surface area, volume, etc.

Typical of method (c) is tomography which uses internal “probing” or “interrogation” followed by “reconstruction” of the volume of the body. The “probes” can include X-rays, gamma rays, magnetic resonance imaging (MRI), and acoustic methods. The results from such scans can be represented as a list of values (x, y, z) which are deemed to be the (central) coordinates of all elements inside the body. If additional properties are measured simultaneously (e.g., density, color), then the list becomes a higher dimensional array. Frequently, the computer is programmed to produce an image of the body which can be manipulated (e.g., magnified, rotated) to serve the needs of the user.

There are extensive bibliographies in all these fields and only a representative few are included in the references.

5. Proposed definitions of size and shape for a single particle

The possibilities generated by these devices suggest the following definitions and procedures to characterize size and shape quantitatively.

Assume that the geometry of a particle has been obtained in discrete numerical form by, for example, tomography. For the present, limit the discussion to bodies that are homogeneous. For simplicity, assume that both the relative density and the acceleration due to gravity are unity. Hence, the weight of the body will be numerically (but not dimensionally) equal to its mass, and weight will be proportional to both mass and volume.

The mathematics will be expressed in rectangular (rather than polar) coordinates and scalar (rather than vector or tensor) form. All these restrictions can be removed but are ignored here for clarity of presentation.

Assume a rectangular coordinate system with origin O and axes x, y, z . Let the entire space of interest be (conceptually) divided into a 3-D array of small cubical elements termed voxels. Assume that the space contains a particle; call it A . Assign a four-member array to each voxel. The first three members of this array are the three spatial coordinates (x, y, z) of its center. The fourth

member, m , is binary: if the tomograph shows that the voxel contains space (air) then set $m=0$. If the voxel contains matter (i.e., the voxel is part of A) set $m=1$. Let there be $p \times q \times r$ voxels in the space.

Then, all the (geometrical) knowledge of the space (and of the body) is contained in the four-dimensional array (x_i, y_i, z_i, m_i) which contains (pqr) members. The geometry of the particle A is defined by the subset of pqr for which $m=1$.

5.1. Size

The size of A can now be defined as the “number of voxels in A ”: this is simply the number of voxels for which $m=1$. Let this be NA . Hence, the size (volume) of A is equal to NA (or NA standard volumes).

An advantage of this system is that it permits a “natural” control of precision: for example, if it is desired to know the size of a body to one part in one thousand, then the space should be divided accordingly (if the measuring device will permit).

5.2. Shape

Shape is now defined as “the spatial distribution of the matter in A ”. In a strict sense, this means that every particle has a unique shape (it being extremely unlikely that any two real particles will be perfectly congruent).

It is, thus, necessary to search for quantitative parameters that can characterize the spatial distribution of voxels. It is proposed to use moments.

6. Review of moments (and sums of moments)

The moment of an element of volume dV about any axis $a-a$ is defined by

$$\text{Moment of } dV \text{ about } a-a = dV \cdot q_a$$

where q_a is the perpendicular distance from [the center of] dV to the axis $a-a$; hereinafter just “the distance from dV to $a-a$ ”.

The moment of a body (i.e., more than one element) is simply the sum of the moments of its component unit volumes (voxels)

$$\text{Moment of body } A \text{ about } a-a = \text{Integral}\{(dV \cdot q_a)\} \text{ or } \sum (dV \cdot q_a)$$

where the sum is computed for all voxels contained in A . The discrete form will be used hereinafter.

It is possible to define and to construct an (infinite) series of such moments by raising the distance term to a power greater than one; thus,

$$m\text{th moment of body } A \text{ about } a-a = \sum [(dV \cdot (q_a)^m)]$$

for all voxels in A .

The moments may be taken about any chosen axis, but one popular choice for axes is described below.

7. Use of first moments: the centroid

For every body, there is a unique point termed the centroid (or center of volume) whose coordinates X , Y , Z (in any selected Cartesian coordinate system) are defined by $X = [\sum(dV*q_x)/\sum(dV)]$ and similarly for Y and Z .

The centroid may be regarded as the geometrical center of the body. If the body possesses any lines or planes of symmetry, then the centroid must lie in those lines or planes. This simplifies its determination—especially if this is performed by hand. For example, if there are three planes of symmetry, the position of the centroid is determined immediately as their common point of intersection. The centroid may lie outside the body (e.g., an annulus).

8. Use of second moments

Of the infinite set of moments available, most previous work (in engineering, at least) has involved second moments (of mass, of volume, and of area). In mechanics, second moments of mass are termed moments of inertia (since they play a central role in the dynamics of bodies; they also occur in most theories of bending in beams). The computation of second moment of volume is very similar. Second moments will be used hereinafter, although the author believes that first moments may offer some computational advantages with no loss of usefulness (e.g., Ref. [1]). This will be explored in a future paper.

When second moments are employed, it is possible to define another type of moment which uses mixed coordinates: these involve two axes rather than one, and are termed product moments.

9. Product moments

Product Moment of body A w.r.t. axes x and y

$$= \sum(dV*q_x*q_y) \text{ for all elements in A.}$$

Product moments can be negative, zero, or positive. The zero case is related to the following important result.

10. Principal axes

It can be shown (e.g., Ref. [7]) that for every body, there exist three special axes which have the following properties;

- (a) they pass through the centroid,
- (b) they are orthogonal,
- (c) their first products of volume are zero.

These axes are termed the principal axes of the body.

The centroid and the three principal axes are commonly employed as the “natural” reference system for the particle.

Thus, for example, if second moments are computed about the principal axes, the results are termed the principal second moments. When ranked numerically, they are termed the maximum, intermediate, and minimum principal second moments and denoted PM1, PM2, and PM3, respectively. All future references to moments herein will mean principal moments unless indicated otherwise.

From the three principal values, it is possible to determine the second moments of the body about any other axes in space.

In summary, every body possesses a centroid and a set of principal axes which may be used as a convenient reference coordinate system for computing moments.

11. Computation of (second) moments and determination of principal axes

When a particle is scanned, the device will have its own coordinate system and it is unlikely that the principal axes of the particle will be coincident with those of the device. Hence, it is necessary to be able to take the moments, which are computed in the device-frame, and compute from them (a) the position of the centroid and (b) the orientation of the principal axes of the particle. Once this is done, all future calculations may be made in the particle's principal axis system. The steps proposed are outlined below.

(1) The body is scanned: the result is a four-dimensional array of the type $(x \ y \ z \ m)$ described above. Solid elements are those for which $m=1$. The xyz coordinate system is that of the scanning device.

(2) The centroid is calculated

$$X = \sum(dV*q_x)/\sum(dV) \text{ similarly for } Y \text{ and } Z$$

(sum is for all solid elements).

(3) The second moments of volume are computed in the (xyz) system.

Second M of volume about $x - x \equiv M_{2xx}$

$$= \sum [(dV)*(q_x)^2]$$

for all voxels in A.

Similar for M_{2yy} and M_{2zz} for y and z axes.

(4) Compute product moments M_{2xy} , M_{2yz} , and M_{2zx} (note $M_{2ij} = M_{2ji}$).

Example $M_{2zx} = \sum [(dV)*(q_z)*(q_x)]$ for all voxels in A.

(5) With the nine moments thus computed, construct the matrix

$$\begin{matrix} M_{2xx} & M_{2xy} & M_{2xz} \\ M_{2yx} & M_{2yy} & M_{2yz} \\ M_{2zx} & M_{2zy} & M_{2zz} \end{matrix}$$

(6) It may be shown (see e.g., Ref. [7]) that the solution of the set of equations

$$\begin{pmatrix} (M_{2xx} - Q) & -M_{2xy} & -M_{2xz} \\ -M_{2yx} & (M_{2yy} - Q) & -M_{2yz} \\ -M_{2zx} & -M_{2zy} & (M_{2zz} - Q) \end{pmatrix} = 0$$

will result in three roots for Q and these are the three principal moments: call them PM1, PM2, and PM3.

(7) It remains to find the directions of the principal axes. Let each axis in the xyz system have direction cosines l_i , m_i , and n_i , where i can take on three values corresponding to the maximum, intermediate, and minimum principal moments. These triads may be found by substituting PM1, PM2, and PM3 (in turn, as PM) in the equation sets below.

$$\begin{pmatrix} (M_{2xx} - PM)*l & -M_{2xy}*m & -M_{2xz}*n \\ -M_{2yx}*l & (M_{2yy} - PM)*m & -M_{2yz}*n \\ -M_{2zx}*l & -M_{2zy}*m & (M_{2zz} - PM)*n \end{pmatrix} = 0.$$

If desired, only two solutions need to be computed because it is known that the principal axes are orthogonal. Hence, $l^2 + m^2 + n^2 = 0$; therefore once any two of $(l, m, n)_i$ are computed, the third may be found from this relationship. However, most computer programs will solve for all three automatically.

(8) An alternative numerical approach (which has not been fully explored at the time of writing) for the determination of the orientation of the principal axes is suggested by the fact that the product moments are zero if taken about the principal axes. Thus, if the moments are first computed in the device frame of reference, the axes may then be rotated by fixed amounts and the product moments recomputed at each step. The principal axes will be found (on the three occasions) when the product moments are zero. Since a true zero will rarely be found exactly, a numerical minimization scheme would need to be developed. It should be a simple task to determine which approach is the more efficient computationally.

At the conclusion of this procedure, a single particle will be “defined” by a quartet of numbers which we may present as

$$(S \text{ PM1 PM2 PM3}).$$

The first number (S) is the number of voxels in the body and measures the size or volume of the particle. The other terms give the principal moments (here, second) for the body. These three numbers provide a numerical measure of the spatial distribution of the matter in the particle, i.e., the shape. Since the shape of the particle is really the entire geometric arrangement of its voxels in space, its replacement by just three quantities may be criticized. While this is true, it may also be noted that every voxel has contributed to each of the three shape numbers.

A second concern is that moments are affected by the size of the body.

11.1. Removing size dependence: normalized moments

A single particle has been characterized by its quartet. It is natural to wish to compare two (and then more) particles. Sizes are easily compared. However, attempts to compare shapes by comparing moments will be complicated by the fact that the numerical value of these terms is size-dependent. This influence of size may be removed by comparing the ratios of the moment terms or, equivalently, as follows. Take each shape term and divide it by the size of the body.

Thus, the final form suggested for characterization of a single particle is

$$(S \text{ PM1/NA PM2/NA PM3/NA}).$$

For brevity in what follows, let these normalized values be written as the quartet

$$(S \text{ N1 N2 N3}).$$

This quartet will permit the comparisons of shape terms for particles without regard to size, when this is necessary or desirable.

Comparisons of shape are further facilitated by Mohr's graphical representation for second moments.

11.2. Mohr's graphical representation of second moments

Mohr [8] discovered that second moments may be described graphically in a circular form now known as Mohr's circle. In 3-D, there are three circles and once these are known, all other second moments (both regular and product) can be found directly. It is usual to show the circles in principal axes space as shown in Fig. 2. Note that the entire set of possible moments is defined by the three quantities N1, N2, N3.

11.3. Application to multiple particles: statistics

In the real world, it is common to deal with assemblages containing billions of particles. It is impractical to attempt to

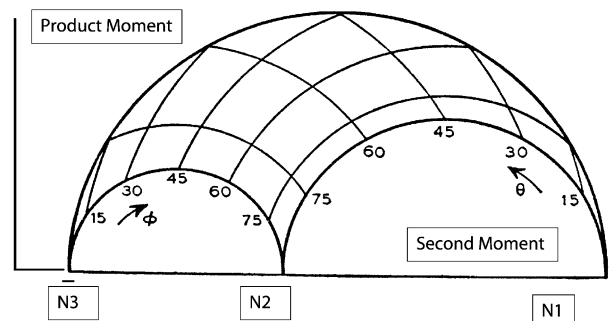


Fig. 2. Using Mohr's Circle and N1, N2, and N3, the two moments can be found graphically for any axis which makes angle θ with the x axis and ϕ with z axis. After Jaeger [4].

Table 1
Second moments of volume for some common shapes

Shape	Major axis		Intermediate		Minor	
	Actual	Normalized	Actual	Normalized	Actual	Normalized
Sphere Diameter = D	$\pi D^4/32$	$3D/16$	$\pi D^4/32$	$3D/16$	$\pi D^4/32$	$3D/16$
Cube Side = D	$D^4/4$	$D/4$	$D^4/4$	$D/4$	$D^4/4$	$D/4$
Block Sides $2D, D, D$	$2*D^5/3$	$D^2/3$	$D^5/12$	$D^2/24$	$D^5/12$	$D^2/24$
Ellipsoid *	$4\pi(a^2 + b^2)*(abc)$	$(a^2 + b^2)/5$	$4\pi(a^2 + c^2)*(abc)$	$(a^2 + c^2)/5$	$4\pi(b^2 + c^2)*(abc)$	$(b^2 + c^2)/5$

* Semi-axes a, b , and c .

scan every particle in such an assemblage: consequently, the use of statistics is indicated. The following is suggested.

A number of particles are sampled from the source to be evaluated. The number needed is dependent upon the level of confidence required by the user. Statistical tables are available to assist in this computation. Suppose that n rocks are scanned by tomography and that, for illustrative purposes, the second moments are of interest.

After computation in principal space, each rock will produce a quartet ($S\ N1\ N2\ N3$) as described above. Let each rock be labeled with an identifier (i) so that its characterization quartet is ($S(i)\ N1(i)\ N2(i)\ N3(i)$). There are n such quartets and so each of the four members of the quartet will have a mean and a standard deviation. Hence, the sample (assemblage) of particles may be characterized by the octet,

($Ss\ NX\ nx\ NY\ ny\ NZ\ nz$)

where the uppercase letters represent the means of the quantities and the lowercase terms represent the standard deviations of the uppercase terms.

This octet is proposed as a quantitative estimate of the properties of the rock population.

12. Discussion and applications

Almost all real world particle are three-dimensional. Hence, definitions of size and/or shape that use only one or two measurements are inadequate. The definitions proposed here offer improved methods for characterization of particles and assemblages of particles. The accumulation of data may be performed by equipment which is presently

available, and the data so obtained is in digital form, which makes the computations suggested here straightforward. The collection of this data may require a significant investment of resources but the data can be used indefinitely into the future (as long as the operating characteristics of the system which produces the particles does not change significantly). If additional evaluations are performed periodically, the database increases in size and scope and the user acquires increased confidence in the results.

For second moments, the Mohr presentation shows that the three principal values $N1, N2$, and $N3$ are sufficient to determine the moments about all other axes, i.e., the solution is unique. This is a powerful attribute of the method. However, other moments may offer advantages and should be explored.

A few representative regular particles and their representations are shown in Table 1 and Fig. 3.

The Mohr circles for all particles which have three axes of symmetry degenerate to a point (although each shape will have a different value for the numerical position of its point, see Fig. 2). The normalized points can distinguish among all such shapes.

Note that the new method will correctly discriminate among the members of Fig. 1.

13. Suggestions for future research

Some possible applications of this approach include comparisons of (a) shapes from different geological sources, (b) shapes produced by different crushing techniques or machines, (c) shapes of products from different sieve fractions for a single geological source, (d) shapes resulting from different feed sizes. Further applications include (e) estimation of the number of contact points in a mass of soil, a catalytic bed, a superconductor, a sintering mass, or a pharmaceutical tablet as these are affected by size and shape and (f) studies of voids, void structures, and permeability in particulate masses.

The usefulness of this proposed system may easily be examined by obtaining tomographic measurements on a representative number of real particles from at least two sources for which some field behavior has been correlated with shape and size. It is hoped that this research will be conducted in the near future.

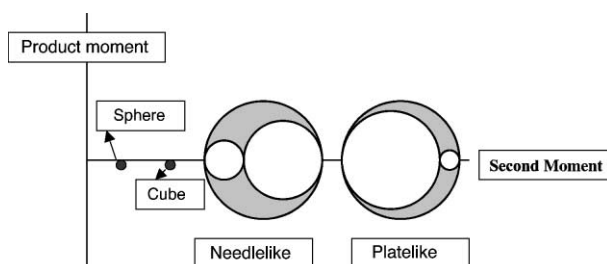


Fig. 3. Appearance of Mohr's Circles for some regular shapes.

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