

Particle Shape Factors and Their Use in Image Analysis—Part 1: Theory

Eric Olson

Fine particles are often characterized by their particle size and distribution as determined by various analytical instruments. Particle shape may be just as important as particle size. Particle shape, however, is often ignored or disregarded. Image analysis is a technique capable of measuring particle shape factors and providing valuable information. These shape factors may dictate the behavior of a product or correlate to a response of interest. Like all measurement techniques, there are limitations and possible sources of error that must be considered when performing particle shape analyses.

INTRODUCTION

Fine particle characterization is most effective when accomplished through a methodical process. The first step of this process often involves determining what material needs characterization. In general, the following instances are most often cited:

- When a new chemical entity or active pharmaceutical ingredient is identified
- When the production of an existing substance is changed (e.g., new salt form established, recrystallization process changed, milling parameters altered, etc.)
- When there exists two lots or batches of virtually identical material that behave differently in some manner.

The process for characterizing these types of materials will vary between companies and probably be dependent on the availability of equipment and the expertise of the associated departments.

Fine Particle Characterization

The first step in fine particle characterization is to observe the particles under a microscope. The importance of this step must be emphasized. Depending on the size and chemical nature of the particles, one may choose various types of microscopy such as brightfield, darkfield, polarized light, phase contrast, etc. The next step may be to get higher magnification and resolution images of the particles through use of scanning electron microscopy (SEM) or transmission electron microscopy (TEM). The wealth of information obtained through microscopy alone should not be underestimated.

The next steps are often conducted in parallel. They include some type of surface area and porosity measurement, as well as particle size, distribution, and shape measurement. The most common type of surface area measurement uses nitrogen gas as the adsorbate and attempts to fit the data with either a Brunauer-Emmett-Teller (1) (BET) or Langmuir (2) model. Likewise, porosity of micropores and mesopores are often measured using gas adsorption and a model such as Barrett-Joyner-Halenda (3) (BJH). Some mesopores and macropores are measured using mercury intrusion porosimetry with the Washburn equation (4).

With regards to particle size measurement, the most common cited statistic is a linear dimension of central tendency, most often of an equivalent circle or sphere (i.e., the mean, median, or mode equivalent spherical diameter of a particle size distribution). Additionally, there are common measurements that are related to the width and shape of the distribution including D_{10} , D_{50} , D_{90} , span, skewness,

kurtosis, standard deviation, and so on. All the aforementioned measurements are made under a set of assumptions for each measurement technique. One common assumption is that the particles are smooth spheres. Thus, there is no shape or texture data associated with these measurements. Furthermore, because the particle shape is assumed spherical, the measured diameter is always equivalent, regardless of particle orientation. In actuality, very few particle types are spherical. Because of this, particles will orient themselves along their respective axes of rotation, and the linear measurements along these axes will no longer be equivalent. This is the primary reason a single linear measurement may not be adequate to describe a typical non-spherical particle with some non-zero degree of surface roughness or a low aspect ratio.

SHAPE FACTORS AND COMPLIANCE

The need for shape determination is stated in the *United States Pharmacopeia (USP) <776> Optical Microscopy* (5), *British Pharmacopoeia Appendix XVII O. Optical Microscopy* (6), *Pharmacopoeia Europe method 2.9.37* (7), and *Japanese Pharmacopoeia, 3.04 Particle Size Determination* (8). They all state, “For spherical particles, size is defined by the diameter. For irregular particles, a variety of definitions of particle size exist. In general, for irregularly-shaped particles, characterization of particle size must also include information on the type of diameter measured as well as information on particle shape.”

One interpretation of this statement is that for particles that are non-spherical or irregularly shaped, the use of image analysis to determine particle size and shape information may be warranted. Time constraints and budget considerations may limit the usage of image analysis especially in a high-throughput setting, so the technique will probably never usurp faster analyses such as laser diffraction or sieving. However, there may be situations where a single particle size value is insufficient to properly characterize a material, especially when multiple lots of the same material exhibit different behaviors.

IMAGE CAPTURE AND CONVERSION

At the core of most image analysis systems is some type of compound microscope. Thus, the process of image analysis inherits most of the issues associated with microscopy. For instance, one of the limitations of image analysis hardware is the ability to not only disperse a sample such that the probability of particles touching is minimized, but also the ability to optically resolve the particles. As one may expect, if two particles are not optically resolved, the resulting image would treat them as a single particle biasing the size results large as well as adversely affecting the shape measurement.

In optics, the resolution, R , is approximated by:

$$R = \frac{0.61\lambda}{N.A.} \quad [\text{Equation 1}]$$

Where λ is the wavelength of the light (0.4 μm is commonly used as an example), and $N.A.$ is the numerical aperture of the lens system. The best way to ensure adequate resolution is to use the appropriate magnification with a suitable numerical aperture. Table I provides a list of the objectives commonly used on the image analysis system called the Malvern Morphologi G3 and their respective sizing limits.

Once an adequate dispersion has been prepared, the proper objectives chosen, and proper focus of the particles has been accomplished, the data capture process can begin. Whether the image analysis is static or dynamic, the process involves taking a two-dimensional image of a three-dimensional particle (9,10). This is an important point because in many types of particle size measurements, the particles are generally free to rotate or translate at will. In the case of dynamic image analysis, the presentation of the particles to the detection optics may depend on the flow rate, viscosity of the diluents, the thickness of the sample holder or aperture, and other parameters. In the case of static image analysis, the particles will generally present themselves with their largest cross-sectional area perpendicular to the light and detection system. Thus, the image analyzed by the detection system is that of the largest cross-sectional projection.

TABLE I: Typical optical resolution of various Malvern Morphologi G3 microscopic objectives.

Magnification	N.A.	R (μm)
2.5x	0.075	3.25
5x	0.15	1.63
10x	0.30	0.81
20x	0.40	0.61
50x	0.55	0.44

Another limitation that image analysis inherits from microscopy is related to contrast. Contrast is defined as the difference in light intensity between the image and the adjacent background relative to the overall background intensity. The observed light intensity is a function of the angle, intensity, and wavelength of the incident light. It is also a function of the refractive indices of both the particle and its surroundings. In general, the contrast will increase as the difference in refractive index between the particle and its surrounding increases. The ratio of the two refractive indices is sometimes referred to as the relative refractive index. Conversely, it is possible to disperse a particle in a diluent in which both have equivalent refractive indices. This is known as refractive index matching, which reduces the contrast to zero, effectively making the particle invisible in its matched diluent. In situations where contrast is less than ideal, it is a common mistake for the threshold to be set too high, leading to dilation (to be discussed). Care must be taken to ensure this does not happen. There are several avenues that can be taken to improve contrast in these cases such as use of a diluent with a different refractive index and use of a stain or dye.

Image, Intensity, and Thresholding

Once the image of a particle is captured by a camera or charge coupled device (CCD), it is digitized into pixels. In this application, a pixel is defined as the smallest unit of light, often rectangular or square, from which images on a television screen or computer monitor may be constructed. Each pixel contains

two types of information: location and intensity. Depending on the quality and style of the camera or CCD, the image may be in color or in black and white (known as grayscale).

In most systems, the grayscale is defined by the intensity of white light. An intensity value of zero indicates there is no white light; hence, it is black. Likewise, a value of 255 indicates a white light of the highest intensity. Therefore, all values within the range from zero to 255 can be thought of as shades of gray. For instance, a value of 150 may be considered “light gray,” while a value of 100 may be considered “dark gray.” Note these values assume a scale from zero to 255. Other scales do exist (e.g., 0 to 63 as shown in Figure 1, 0 to 127, or more rarely 0 to 511).

The manner by which the edge of a particle is defined is commonly referred to as thresholding. By thresholding, one defines the threshold by which when surpassed, the edge of a particle is indicated. For example, if the intensity value of the background of an image is measured as 150 (“light gray”) and the threshold is chosen to be 100 (“dark gray”), then anywhere in the field of view where the pixel intensity value exceeds 100 is considered the edge or interior of a particle.

Thresholding is a process that may lead to biased data. Figure 2 is an image illustrating when the thresholding is set too low (known as erosion). Closer examination of Figure 2 shows how the outline or edge of the particle is very irregular. In addition, the edge of the particle is clearly within the circular band around the particle that is the darkest. As the threshold is decreased, more of the actual particle edge is eroded, hence the term. Because erosion eliminates pixels from the actual particle edge, the overall effect is a bias of the data towards the smaller size. It may also affect certain shape measurements defined later in this paper.

Ideally, the edge of the particle should be dark and relatively smooth as shown in Figure 3. There should be no lighter halo around the edge, and likewise, there should be no evidence of erosion.

Figure 4 illustrates thresholding set too high (known as dilation). As demonstrated in Figure 4, it is clear there is a lighter colored ring or band, some-

Figure 1:

A grayscale from white (63) to black (0).

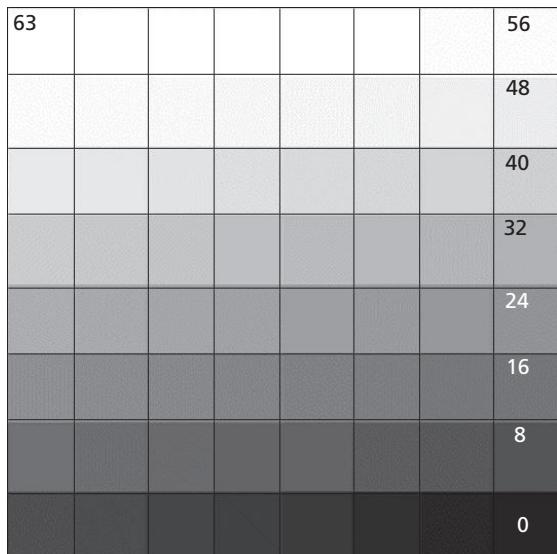


Figure 2:

Erosion of a glass sphere (threshold = 50).

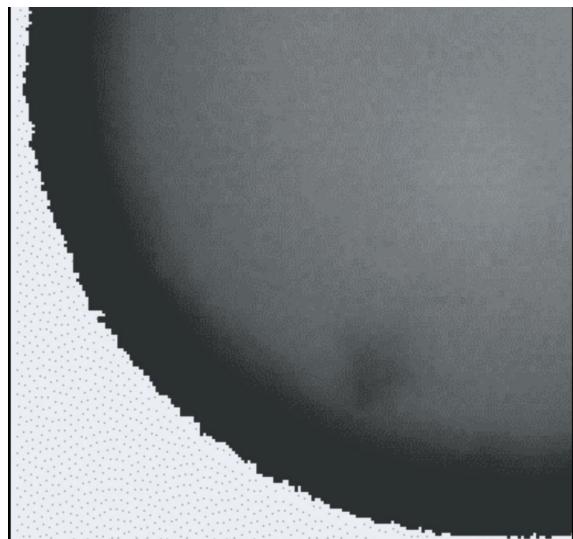


Figure 3:

Proper threshold of a glass sphere (threshold = 100).

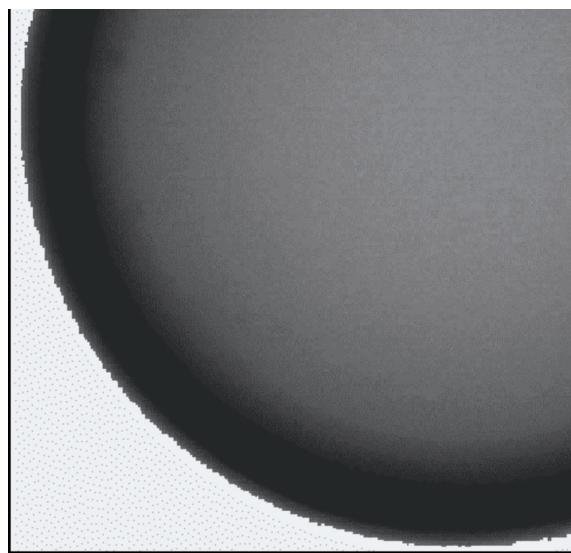
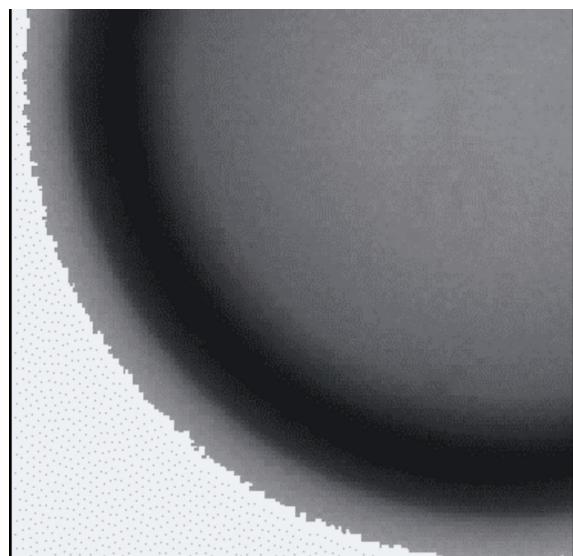


Figure 4:

Dilation of a glass sphere (threshold = 150).



times called a halo, around the edge of the particle. It is sometimes irregular as in this case, but not always. As the threshold is increased, the thickness of the halo will typically increase. The overall result of dilation is to bias the data towards the larger size.

In most cases, the threshold is chosen manually and, thus, is prone to human error and subjectivity. One way to decrease this error is to choose a constant threshold for all fields of view. Setting the threshold is generally not very difficult but does require that the background be a consistent intensity or grayscale value. This is accomplished by automatically measuring and adjusting the incident light intensity to a constant value prior to every analysis and sample preparation, which is common in modern static image analysis systems. However, it is one of the more challenging feats to accomplish when using fully manual instrumentation.

Shape Measurements

Once an image of a particle has been obtained and digitized and the edges of each particle have been defined, it is then possible to begin making shape measurements. In order to ensure the measurements are accurate and reproducible, the instrument must be calibrated. This is most often accomplished through use of a National Institute of Standards and Technology (NIST) traceable stage micrometer or similar set of gratings. In practice, an image of the micrometer is taken at the same magnification and lighting level as used for the particulate analysis (see Figure 5). The software then measures the distance between the gratings of the micrometer in units of pixels. If the actual distance between the gratings is known, a calibration constant can be generated, which is most often expressed in units of pixels per micron. With this calibration constant, all shape and size measurements can be made in units of pixels and then converted to a more useful unit such as microns.

Calibration of the system is of great importance. For this reason, it is highly suggested that a NIST traceable stage micrometer or similar certified device be used. If possible, this should be done automatically, thus eliminating the possibility of human inter-

pretation and bias. As expected, the level of error in the system can be relatively large when using higher magnification objectives. In fact, calibration of the system at the highest magnification levels may need to take place more than once a day to ensure optimum accuracy due to slight changes in laboratory temperature and thermal expansion of the optics.

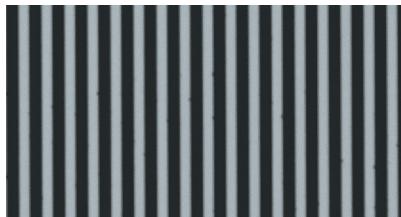
ISO 13322-1 has a very detailed derivation and description of how to calculate the minimum number of particles necessary to ensure a statistical confidence level (9). The method is beyond the scope of this paper, but the minimum number is a function of the geometric standard deviation of the particle size distribution, whether the distribution is presented on a count or mass basis and the level of admissible error. One of the most common errors committed when conducting image analysis is to collect too few images, especially if the system is manual rather than automated. For example, for data presented on a count basis at the 95% confidence level, the minimum number of images required with a geometric standard deviation of 1.40 is about 19,000. As the geometric standard deviation increases to 1.50 and 1.60, the minimum number of images required is approximately 36,000 and 61,000, respectively. As shown by these examples, as the geometric standard deviation increases, the number of required particles increases quite rapidly. Broad distributions with a geometric standard deviation in excess of 2.0 or even 2.5 are not unexpected in fine particle analysis. The number of required images for broad distributions such as those quickly reaches hundreds of thousands if one is to maintain a reasonable confidence level.

SHAPE FACTOR DEFINITIONS

There are many ways to subdivide and categorize the basic types of measurements used in image analysis. These terms vary depending on the source. One common way to categorize the types of measurements is based on scale. The largest scale measurements are sometimes referred to as form, which reflects the geometric proportions of the particle. The next smaller scale measurement, roundness, expresses the radius of curvature of the particle corners. Finally, the smallest scale measurement,

Figure 5:

Image of NIST traceable stage micrometer at 200x magnification.



roughness, is representative of local surface texture between corners.

Another way to categorize the types of measurements is based on the level of assumptions and the degree to which the results are calculated. For instance, the area, perimeter, and most linear results are direct measurements from the image pixel map. From these, various results such as the circular equivalent diameter and spherical equivalent volume are calculated. Finally, using various equations and ratios of the aforementioned factors, responses such as the aspect ratio, circularity, convexity, and solidity may be calculated.

The list of definitions discussed below is by no means exhaustive, but is rather a combination of parameters used in Image Pro Plus (Media Cybernetics) and the Malvern Morphologi (Malvern Instruments Ltd) software packages (11, 12). Other measurements (e.g., the fractal dimension, concavity, diameter of the maximum inscribed circle, geodesic length, geodesic thickness, elliptical shape factor, elongation, straightness, irregularity, compactness, roundness, extent, robustness, etc.) are sometimes used and referred to in the literature (13-20). Often, the choice of shape factors is dependent on the nature of the questions being asked, the particles in question, and to some extent, the particular field of study in which the particles are being used.

Area

Most often, the first measurement is the projected two-dimensional area, A . The area of the particle is calculated as the sum of the areas of each individual pixel, a_p , within the borders of the particle per Equation 2. Note the units of A are in pixels (2), but as-

suming the system has been calibrated with a stage micrometer, the area may then be converted to units of μm^2 .

$$A = \sum a_p \quad [\text{Equation 2}]$$

Circular Equivalent Diameter

The circular equivalent diameter, or area-equivalent diameter, is defined as the diameter of a circle with the same area as the particle. Thus, once the area of the particle, A , has been measured, the area-equivalent diameter (x_A) can be calculated per Equation 3. It is most often expressed in units of μm .

$$x_A = \sqrt{\frac{4A}{\pi}} \quad [\text{Equation 3}]$$

Spherical Equivalent Volume

Like the circular equivalent diameter, the spherical equivalent volume, V , is defined as the volume of a sphere whose diameter is a function of the measured area:

$$V = \frac{1}{6}\pi \left(\sqrt{\frac{4A}{\pi}} \right)^3 = \frac{1}{6}\pi (x_A^3) \quad [\text{Equation 4}]$$

Feret's Diameters

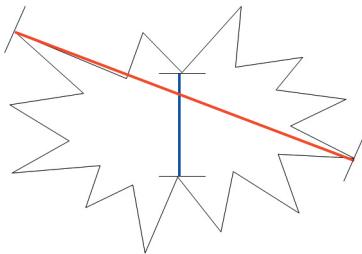
The maximum Feret's diameter, $x_{F_{\max}}$, also called the maximum distance in some references, is defined as the furthest distance between any two parallel tangents on the particle. Likewise, the minimum Feret's diameter, $x_{F_{\min}}$, also called the minimum distance in some references, is defined as the shortest distance between any two parallel tangents on the particle. The units for the Feret's diameters are most often expressed in μm . These are illustrated in Figure 6.

Major and Minor Axes

All particulate matter has major and minor axes. The major axis passes through the center of mass of the object corresponding to the minimum rotational energy of the shape. The minor axis passes through the center of mass of the object and is always perpendicular to the major axis. The major and minor axes are

Figure 6:

Maximum Feret's diameter, x_{Fmax} (red), and the minimum Feret's diameter, x_{Fmin} (blue).



illustrated as dotted lines in Figure 7. Note the major axis is expressed in units of degrees that it deviates from a horizontal line. Because the minor axis is perpendicular, it will always be the angle of the major axis + 90°. In Figure 7, the major axis was measured as 68°, and the subsequent minor axis was 158°.

Length and Width

The length is the maximum distance between any two points on the perimeter of the particle parallel to the major axis. Likewise, the width is the maximum distance between any two points on the perimeter of the particle parallel to the minor axis. The units for length and width are most often expressed in μm . The length and width are illustrated in Figure 7.

Perimeter

The perimeter of the particle, P , is defined as the total length of the object boundary. The perimeter is calculated per the Cauchy-Crofton equation (Equation 5), from the number of intercepts, I , formed by a series of parallel lines, with spacing d_L , exploring N directions, from α to π . The units of the perimeter are most often expressed in μm .

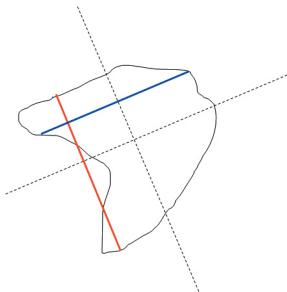
$$P = \frac{\pi}{N} \sum_{\alpha} I_{\alpha} d_L \quad [\text{Equation 5}]$$

Convex Hull Perimeter

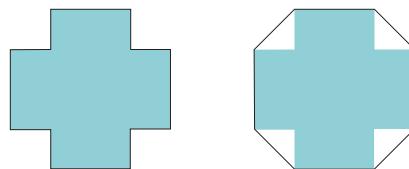
The convex hull of a particle can be thought of as the particle surrounded by a rubber band. It is sometimes also referred to as a convex envelope or simply as an envelope. Figure 8 illustrates the difference be-

Figure 7:

A particle indicating the major and minor axes (dashed lines), as well as the length (red) and width (blue).

**Figure 8:**

Perimeter (left) and convex hull perimeter (right) of an equivalent shape.



tween a perimeter, P (left) and a convex hull perimeter, P_c (right). The units of the convex hull perimeter are most often expressed in μm . Note the equivalent shapes are blue, while the respective perimeters are indicated by the black lines.

Convex Hull Area

The convex hull can also be used to calculate the respective convex hull area, A_c as illustrated in Figure 9. The units of the convex hull area are most frequently expressed in μm^2 . Note the respective areas of the equivalent shapes are indicated by the black figures.

Aspect Ratio

Aspect ratio has been previously defined several ways and is a function of more than one factor. Aspect ratio has been used historically to classify the general form of particles (e.g., equant, acicular, or fibrous). Most of the older literature calculated aspect ratio as length divided by width. In some fields such as clays and micas, aspect ratio has even been defined as area divided by particle thickness. More recently, ISO 9276-6 defines the aspect ratio as the ratio of

Figure 9:

Area (left) and convex hull area (right) of an equivalent shape.



the Feret's minimum length to the Feret's maximum length as given in Equation 6 (21). This is done to scale the aspect ratio such that the value is always in the range, $0 < AR \leq 1$. Aspect ratio is a dimensionless value. Note that ISO 9276-6 expressly states aspect ratio is only for particles that are "not very elongated." Though not discussed in this paper, elongation is defined as $1 - \text{the aspect ratio}$. Thus, though it may be useful for acicular or needle-like particles, aspect ratio is not applicable to elongated particles such as fibers or ribbons. Other shape descriptors and measurements such as the geodesic length and geodesic width are suggested for these shapes.

$$AR = \frac{x_{F \min}}{x_{F \max}} \quad [\text{Equation } 6]$$

Circularity

Circularity, C , is defined as the degree to which the particle is similar to a circle, taking into consideration the smoothness of the perimeter. This means circularity is a measurement of both the particle form and roughness. Thus, the further away from a perfectly round and smooth circle that a particle becomes, the lower the circularity value. Circularity is a dimensionless value. ISO 9276-6 defines circularity per Equation 7.

$$C = \sqrt{\frac{4\pi A}{P^2}} \quad [\text{Equation } 7]$$

Convexity

Convexity, C_x , is a measurement of the particle edge roughness and is defined as the convex hull perimeter, P_c , divided by the actual perimeter, P , as given in Equation 8. Thus, as the surface of the particle becomes rough, the convex hull perimeter increases,

also raising the convexity measurement. Convexity is a dimensionless value.

$$C_x = \frac{P_c}{P} \quad [\text{Equation } 8]$$

Solidity

Solidity, S , is the measurement of the overall concavity of a particle. It is defined as the image area, A , divided by the convex hull area, A_c , as given in Equation 9. Thus, as the particle becomes more solid, the image area and convex hull area approach each other, resulting in a solidity value of one. However, as the particle form digresses from a closed circle, the convex hull area increases and the calculated solidity decreases. Solidity is a dimensionless value.

$$S = \frac{A}{A_c} \quad [\text{Equation } 9]$$

EXAMPLE SHAPES AND DATA

The 23 images given in Figures 10-13 were drawn using Microsoft PowerPoint, then imported and analyzed using the Malvern Morphologi G3S software. The set of images used is certainly not exhaustive, but should provide enough examples across a broad spectrum of shapes to be sufficiently illustrative. The images are presented with their respective particle ID numbers, which will be referenced throughout this section of the paper. The resulting data of the dimensionless shape factors are given in Table II.

OBSERVATIONS AND TRENDS

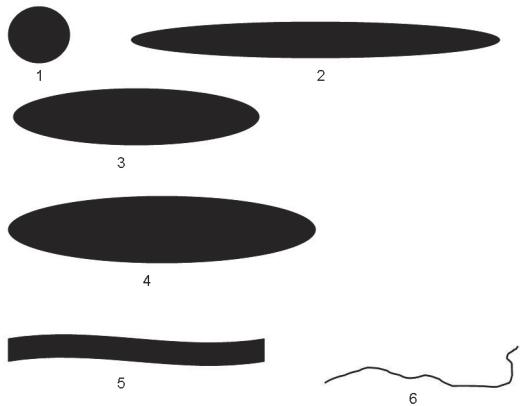
There are many trends observed throughout the data in Table II. These will be discussed on a per-shape-descriptor basis. Note there are some errors associated with the measurements. In this case, the errors are solely due to the author's inability to draw perfect regular shapes with the software tools used.

Aspect Ratio

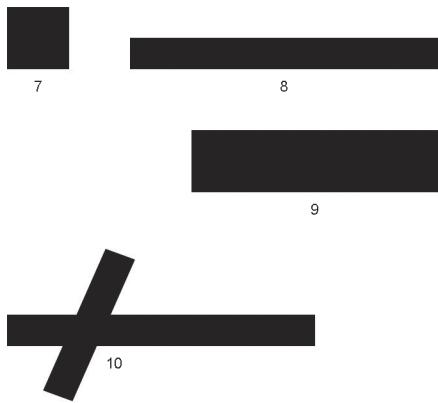
Aspect ratio is defined as the ratio of the Feret's minimum length to the Feret's maximum length as given in Equation

Figure 10:

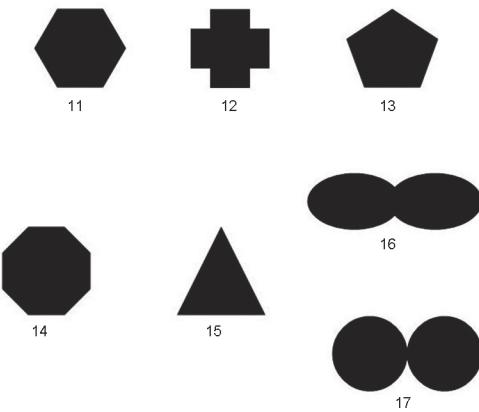
Various shapes, 1 to 6.

**Figure 11:**

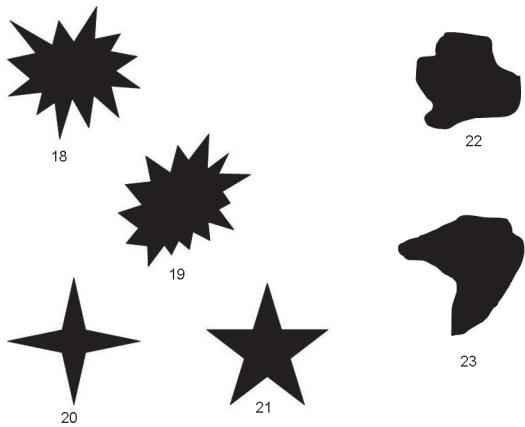
Various shapes, 7 to 10.

**Figure 12:**

Various shapes, 11 to 17.

**Figure 13:**

Various shapes, 18 to 23.



6. Thus, as the width and length of the shape approach the same value, the aspect ratio approaches one. This does not necessarily mean the shape is circular, though a perfect circle does have an aspect ratio of 1.0 (shape #1). Often very symmetric shapes also have a very high aspect ratio. For instance, shapes #7 (square), #12 (symmetric cross), #14 (regular octagon), #15 (equilateral triangle), #21 (5-point star), and #20 (4-point star) all have aspect ratios >0.95 as measured in this example.

The converse of this is also true. Thus, as the measure-

ments of the width and length of the shape diverge, the aspect ratio approaches zero. Examples of this are given by shapes #2 (torpedo shape), #8 (long rectangle), #5 (ribbon), #6 (fiber), #3 and #4 (ellipses), and #9 (medium rectangle), which all have aspect ratios ≤ 0.25 as measured in this example.

Two shapes of further interest are #17 (two touching circles) and #10 (two intersecting rectangles). Shape #17 is of interest because from a geometric point of view, the width should be one diameter and the length should

TABLE II: Analysis of various shapes—dimensionless shape factors.

ID	Shape Description	Aspect Ratio	Circularity	Convexity	Solidity
1	Circle	1	1	1	1
2	Torpedo	0.10	0.49	1	1
3	Long ellipse	0.22	0.69	1	1
4	Medium ellipse	0.23	0.71	1	1
5	Ribbon	0.11	0.49	0.99	0.85
6	Fiber	0.20	0.14	0.89	0.10
7	Square	1	0.89	1	1
8	Long rectangle	0.10	0.51	1	1
9	Medium rectangle	0.25	0.71	1	1
10	Twinning	0.49	0.45	0.82	0.47
11	Regular hexagon	0.90	0.95	1	1
12	Symmetric cross	1	0.79	0.87	0.87
13	Regular pentagon	0.86	0.93	1	1
14	Regular octagon	1	0.97	1	1
15	Equilateral triangle	1	0.78	1	1
16	Peanut	0.33	0.77	0.96	0.92
17	Touching circles	0.50	0.75	0.87	0.88
18	Star	1	0.42	0.58	0.59
19	Star	0.81	0.49	0.63	0.69
20	4-point star	0.96	0.45	0.83	0.38
21	5-point star	0.98	0.52	0.81	0.50
22	Random shape	0.94	0.86	0.94	0.91
23	Random shape	0.92	0.79	0.94	0.82

be two diameters. Hence, the aspect ratio should be 0.5, which it was. Shape #10 is of interest because it is a common shape often seen with crystals that are aggregated, which is sometimes referred to as “twinning.” The result of twinning and for most types of aggregation is the measured aspect ratio is larger than that of the individual primary particle. In this

example, shape #10 (twinning) can be compared to shape #8 (long rectangle), in which the aspect ratios were 0.49 and 0.10, respectively.

Circularity

Circularity is a function of the area divided by the square of the perimeter as shown in Equation 7.

Circularity is a measurement of both the particle form and roughness. Thus, one would expect as a shape becomes more round and smooth, the circularity would approach one. This is demonstrated by shapes #1 (circle), and to a lesser extent, #14 (regular octagon). These have circularity values ≥ 0.98 .

Conversely, as a shape becomes less round or as the shape becomes less smooth, the circularity should approach zero. This is demonstrated by shapes #6 (fiber), #18 (star), #20 (4-point star), #10 (twinning), #19 (star), #2 (torpedo), and #5 (ribbon). These all have circularity values < 0.5 . Note the number of examples, which are very elongated, irregular, asymmetrical, or described as some type of star.

Another trend with regards to circularity was observed throughout the regular polygons. As one would expect, as the number of sides of a polygon approaches infinity, the polygon more closely resembles a circle. Thus, as the number of sides of a polygon increases, one should expect the circularity to also increase. This is the case as shown in Table II. In order of decreasing circularity, the regular polygons could be arranged by their number of respective sides: shape #14 (octagon) $>$ #11 (hexagon) $>$ #13 (pentagon) $>$ #7 (square) $>$ #15 (equilateral triangle).

Convexity

Convexity is a measurement of the particle edge roughness and is defined as the convex hull perimeter divided by the actual perimeter as given in Equation 8. When a shape becomes less smooth (or rougher), the perimeter of the shape may increase very quickly depending on the size and number of the irregularities in the shape contributing to the roughness. However, the convex hull perimeter is an envelope measurement. By surrounding or enveloping the shape, the net effect is to smooth the perimeter into the convex hull. Thus, as the shape becomes less smooth, the convex hull perimeter changes at a much slower rate, and eventually approaches a larger but smooth circle. Therefore, as the shape becomes less smooth, one should expect the convexity to approach zero. This is demonstrated by shape #18 (star), #19 (star), #21 (5-point star), #10 (twinning),

and #20 (4-point star). These all had convexity values < 0.85 .

Conversely, as the shape becomes smoother, one would expect the convexity to approach one. This is demonstrated by the 15 shapes with convexity values > 0.90 . This was expected given that so many of the shapes were drawn with completely smooth lines or arcs.

Convexity is very sensitive to surface roughness. Likewise, the specific surface area of a particle is related to the particle diameter, porosity, and surface roughness. Thus, convexity and specific surface area may often be strongly correlated, depending on the mechanism to which the particle may attribute its higher specific surface area.

Solidity

Solidity is the measurement of the overall concavity of a particle. Solidity is defined as the image area divided by the convex hull area as given in Equation 9. If an imaginary rubber band is stretched around a shape forming a convex hull, solidity is the measurement of the area within the convex hull that is filled or solid. Solidity is dependent on the convex hull like convexity. Thus, there are two rates to consider as a shape becomes more or less solid. Those are the rate of change of the actual particle area and the rate of change of the convex hull area. The rate of change of the convex hull area changes at a different rate than the actual area because the process of enveloping the shape in a convex hull has the net effect of smoothing the shape. As a shape becomes rougher or less solid, the solidity value will approach zero. This is demonstrated by shapes #6 (fiber), #20 (4-point star), #10 (twinning), #21 (5-point star), #18 and #19 (stars). These all had solidity values < 0.7 .

Conversely, very smooth rounded shapes had solidity values that approach one. This is demonstrated by the 11 shapes with solidity values > 0.99 . These results, like those for convexity, were expected because both shape descriptors are sensitive to shape roughness, both are related to a convex hull measurement, and because so many of the shapes were drawn with completely smooth lines or arcs.

CONCLUSIONS

A single linear measurement (i.e., circular equivalent diameter) may not be adequate to describe a typical non-spherical particle with some degree of surface roughness. There are various definitions and several standardized shape factors available that can provide additional descriptors to a particle population of interest. These valuable shape descriptors can be measured using image analysis. There are numerous examples of how the shape of the particle may influence its behavior or correlate to a response of interest. Because of this importance, shape factors may be necessary to consider in validated characterization methods. However, like all measurement techniques, there are limitations and possible sources of error. These limitations can be minimized with a thorough understanding of the shape definitions and how they can be used to improve the quality and performance of a material.

REFERENCES

1. Brunauer, Emmett, Teller, *J. Am. Chem. Soc.*, 2, 60, 1938.
2. Langmuir, *J. Am. Chem. Soc.*, 11, 38, 1916.
3. Barrett, Joyner, Halenda, *J. Am. Chem. Soc.*, 1, 73, 1951.
4. Washburn, *Proc. Nat. Acad. Sci.*, 7, 115, 1921.
5. USP, *United States Pharmacopeia*, <776> Optical Microscopy, *USP34-NF29*, 2011.
6. BP, *British Pharmacopoeia*, Appendix XVII O. Optical Microscopy, 2007.
7. EDQM, *European Pharmacopoeia*, Method 2.9.37, DATE?
8. JP, *Japanese Pharmacopoeia*, 3.04 Particle Size Determination, 2006.
9. ISO, ISO 13322-1, "Particle size analysis—Image analysis methods—Part 1: Static image analysis methods," 2004.
10. ISO, ISO 13322-2, "Particle size analysis—Image analysis methods—Part 2: Dynamic image analysis methods," 1996.
11. Malvern Instruments Ltd, *Morphologi G3 User Manual*, 2010.
12. Media Cybernetics, *Image Pro Plus User Manual*, V3, 1997.
13. Russ, *The Image Processing Handbook*, CRC Press LLC, 1998.
14. Mikli, Käerdi, Kulu, & Besterci, "Characterization of Powder Morphology," *Proc. Estonian Acad. Sci. Eng.*, 7, 2001
15. Faria, Pons, Feyo De Azevedo, Rocha, & Vivier, "Quantification of the Morphology of Sucrose Crystals by Image Analysis," *Powder Technology*, 133, 2003.
16. Schmid, Dvorak, Müller, & Müssig, "Characterizing Flock Fibers using Quantitative Image Analysis," *Flock*, 30, 2004.
17. Medalia, "Dynamic Shape Factors for Particles," *Powder Technology*, 4, 1970.
18. Pons, Vivier, Belaroui, Bernard-Michel, & Cordier, "Particle Morphology: From Visualization to Measurement," *Powder Technology*, 103, 1999.
19. Pons, Vivier, & Dodds, "Particle Shape Characterization using Morphological Descriptors," *Part. and Part. Syst. Charact.*, 14, 1997.
20. Kaye, "Characterizing the Flowability of a Powder Using the Concepts of Fractal Geometry and Chaos Theory," *Part. and Part. Syst. Charact.*, 14, 1997.
21. ISO, ISO 9276-6:2008(E), Representation of results of particle size analysis—Part 6: Descriptive and quantitative representation of particle shape and morphology, 2008.

GXP

ARTICLE ACRONYM LISTING

BET	Brunauer-Emmett-Teller
BJH	Barrett-Joyner-Halenda
CCD	Charge Coupled Device
ISO	International Organization on Standardization
NIST	National Institute of Standards and Technology
SEM	Scanning Electron Microscope
TEM	Transmission Electron Microscope

ABOUT THE AUTHOR

Eric Olson is the senior chemist at Particle Technology Labs, Downers Grove, IL, USA. Eric has more than 16 years experience in the fields of fine particle technology, chemistry, and statistics. Eric is a member of the American Chemical Society, ACS Division of Colloid and Interface Science, Society for Applied Spectroscopy, Council for Near-Infrared Spectroscopy, Coblenz Society, and the Federation of Analytical Chemistry and Spectroscopy Studies. He may be contacted at EOLson@particletechlabs.com.