Two-Dimensional Shape and Size Characterization of Polygonally Symmetric Particles

PAO K. WANG

Department of Meteorology, University of Wisconsin, Madison, Wisconsin 53706

Received May 27, 1986; accepted August 15, 1986

A simple mathematical expression with four variable parameters is introduced for the purpose of generating two-dimensional polygonally symmetric shapes. The motivation of the implementation of this expression is to improve the methods of characterization of particle shapes and sizes. Previous methods include the purely size classification, which does not carry information about the shape, and the orthogonal polynomial method, which involves too many parameters and therefore is too complicated. It is demonstrated that the simple equation introduced here is capable of simulating many shapes such as quasi-spherical particles and near-exact polygons. Values of the parameters for generating near-exact polygons are included. A sample of simulated particles is generated by this equation with a predetermined distribution of parameters to show the diversity of the shapes and sizes of particles represented by the equation. Since each parameter has a clear physical meaning (a, amplitude parameter; b, width parameter; c, center size parameter; and n, polygonality parameter), it may be possible to explain the physical processes involved by examining the distributions of each parameter.

1. INTRODUCTION

Shape and size are two parameters that strongly influence the physical and dynamic properties of colloidal particles. For example, it is well known that the scattering of light by particles depends very much on their sizes and shapes (1–3). The collisional and coagulational behaviors are different for particles of different shapes, not only because of their different contact geometry but also because they cause different flow fields. The configurations of electrostatic fields of charged particles will be different if their shapes are different. For example, a charged conducting sphere would show a radially symmetric field. In contrast, a charged conducting finite cylinder would have field intensities concentrated at the sharp edges (4). As a result, the electromechanical behaviors of cylindrical particles will be different from those of spheres.

In addition to its importance in physical and dynamical properties, the information on shape and size distributions is sometimes necessary for describing certain processes, for example, the changes in shapes of particles due to coagulation and the dissolution of certain crystals in an emulsion. Several similar, but not entirely identical, particles may be involved in these processes and their shapes and sizes change with time. It is very desirable to describe these processes quantitatively.

Despite the equal importance of shape and size, the shape factor has rarely been treated quantitatively. The great majority of aerosol studies assume that particles are spheres, even after they collide and coagulate together. This is clearly unsatisfactory. While the conventional method of dealing with nonspherical particles is to define the so-called equivalent spheres, and it certainly serves well as a first-order approximation, it is also true that much information about the particles is lost due to such an assumption. Simple methods of characterizing nonspherical particles are clearly desirable.

This paper is motivated by such a need. The goal of this work is to look for a simple mathematical expression which can represent many common shapes of particles. Highly irregular
particles are not considered as they require more complicated treatments. Specifically we treat here particles of many sides or branches which are arranged in a regular manner. We call them polygonally symmetric particles. One familiar example is a hexagonal crystal which is not radially symmetric but in which the six sectors do arrange in a symmetric way. There are many natural or man-made particles that are polygonally symmetric. As will be seen in the next section, it is possible to use a simple equation to generate these shapes. “Simple” here means that only a small number of parameters in the equation are allowed to vary so that it is meaningful to speak of the classification of shapes and sizes in terms of these parameters. A classification method involving too many parameters is not very meaningful.

The equation presented contains four parameters. It is, however, not always necessary to vary all four parameters at the same time because in many cases particles are of similar (but not identical) shapes and sizes and frequently only two or three parameters need to be varied. This equation is most convenient when this is the case. Examples of the shapes generated by this equation are shown. Some variations of the equation are also discussed.

2. GENERATING EQUATION

The equation introduced here is similar to the two expressions introduced by Wang and Denzer (5) to describe hexagonal snow crystals. The current equation is more general and can generate a wide variety of shapes by varying the four parameters. This equation is, in polar coordinates,

\[ r = a [\sin^2(n\theta)] b + c, \]  

where \( a, b, c, \) and \( n \) are the parameters to be varied in order to fit particle shapes. The ranges of these parameters are

\( a: \) from \(-c\) to \(\infty\) (amplitude parameter) 
\( b: \) from 0 to \(\infty\) (width parameter) 
\( c: \) from 0 to \(\infty\) (center size parameter) 
\( n: \) \(0, 0.5, 1, 1.5, 2, 2.5, \ldots\) (polygonality parameter).

The names of these parameters will become clear in the following discussions. Note that the values of \( n \) do not have to be integers but can be multiples of \( \frac{1}{2} \). This can be seen easily from the fact that the curve generated by Eq. [1] has to close onto itself. This requires that \( r(0) = r(2\pi) \). Therefore from [1]

\[ r(0) = c = r(2\pi) = a[\sin^2(2n\pi)] b + c. \]  

Thus the criterion of self-closing becomes

\[ \sin(2n\pi) = 0, \]  

which demands that

\[ n = m/2, \quad m = 0, 1, 2, 3, \ldots \]  

The minimum value of \( a \) is set at \(-c\) to prevent negative values of \( r \). We also restrict the values of \( b \) to be positive here. The case of negative \( b \) is discussed later.

Equation [1] represents essentially a circle with radius \( c \) modified by the term \( a[\sin^2(n\theta)] b \). The square of the sine function generates a closed waveform with \( 2n \) waves, the width of each wave being regulated by the parameter \( b \). Since \( 0 \leq \sin^2(n\theta) \leq 1 \), the width of the wave decreases with increasing \( b \). The range of \( r \) is between \( c \) and \( a + c \). Depending on whether \( a \) is positive or negative, \( a + c \) can be larger or smaller than \( c \), respectively. Each parameter thus has a special role in the shape and size characterization. We call \( a \) the amplitude parameter, \( b \) the width parameter, \( c \) the center size parameter (which represents the size of the central disk), and \( n \) the polygonality parameter (for a given \( n \), the particle will have \( 2n \) sides or branches).

Once these four parameters are specified, both the two-dimensional size and shape of a particle is completely determined. Other geometrical quantities can be calculated easily from Eq. [1]. For example, the area enclosed by the curve will be given by

\[ A = \frac{1}{2} \int_0^{2\pi} r^2 d\theta, \]  

\[ \text{Journal of Colloid and Interface Science, Vol. 117, No. 1, May 1987} \]
where \( r \) in the integrand is to be substituted by the right-hand side of Eq. [1]. This integration can be calculated easily by either analytical or numerical methods. If the particle is a plate with area \( A \) and thickness \( h \), then the volume is given by \( V = Ah \).

Because Eq. [1] is based on the modification of a circle \( r = c \), the curves have the base of a circle. It can be easily seen that if the circle is replaced by an ellipse, then the curves will have the base shape of an ellipse.

3. EXAMPLES

Figures 1–3 illustrate various shapes generated by Eq. [1]. Figures 1a–2c are curves with \( a > 0 \). In these cases, the smaller the values of \( b \), the broader, or “fatter,” the branches. For example, Fig. 1a shows the shapes with \( b = 0.1, c = 0.3 \), and \( a \) from 0.05 to 0.25. Note that the absolute magnitudes of \( a \) and \( c \) are important to the size but not to the shape. As far as the shape is concerned, only the ratio \( a/c \) is of significance. All the shapes in Fig. 1a have relatively fat branches because of the relatively small value of \( b \). Since \( c \) is fixed, the increasing \( a \) serves to increase the overall size of the particle.

As \( b \) increases, the width of the branches decreases, as it should. This is clearly seen in Fig. 1b. Again, because \( c \) is fixed, the effect of increasing \( a \) is to increase the overall size of the particle. As \( b \) becomes larger than that in Fig. 1a, the branches become sharper. As \( b \) increases even further to 100 (see Fig. 1c) the branches become sharp spikes.

Depending on one’s application, the shapes in Figs. 1a–1c can be used for simulating the shapes of some pollens (e.g., the lowest row of Fig. 1a), or some spiked pollen (the upper row of Fig. 1c), large drops (the lowest row of Fig. 1d), and biological cells in mitosis (the second row in Fig. 1a) (see, e.g., (7)).

In Figs. 1a–1c we have \( a \leq c \) and it is there-
fore quite appropriate to say that \( a[\sin^2(n\theta)]^b \) is a modification of the circle \( r = c \). As the value of \( a \) increases such that \( a > c \), the features of the \( a \) term actually dominate, as seen in Figs. 1d–2c. The shapes in the lowest row of Fig. 1d resemble the shapes of large falling water drops (see (6)). If the values of \( b \) and \( n \) increase, as is the case in Fig. 2a, the \( a \) term becomes a large number of needles dwelling on a circle.

Figures 2b and 2c represent the cases where \( c = 0 \). In these cases all branches are in contact with each other only at the center. Figure 2b represents cases with a small \( b \) value (\( b = 0.1 \)). Figure 2c represents a large \( b \) value (\( b = 100 \)). Note that the uppermost row shapes (\( n = 3 \)) look exactly like the stellar snow crystals.

The values of the amplitude parameter \( a \) in Figs. 1a–2c are positive. The features of \( a \) terms are added to the circle. As mentioned earlier, \( a \) can also assume negative values. In this case, the features of an \( a \) term are subtracted from the circle and therefore represent inward modifications. The effect of \( b \) now becomes the reverse of the positive \( a \) cases, namely, the smaller the \( b \) value, the narrower the branches. Figures 2d–3b illustrate these negative \( a \) cases. In Fig. 2d, sharp spikes are produced. The curvatures of these spikes have signs opposite to those in Fig. 2a because this is an inward modification. Figure 3a contains some shapes that are almost exact polygons, which will be discussed in further detail in the next section. In Fig. 3b, the branches become quite broad due to the larger values of \( b \). The shapes in the lowest rows in both figures are similar to those in Fig. 1d but the patterns are reversed in the left–right direction. These shapes again can simulate large falling liquid drops. Note that the shapes in the upper rows of Fig. 3b can simulate not only planar particles with branches but also the cross sections.

![Fig. 2. Shapes generated by Eq. [1]: (a) \( a = 0.1, 0.3, \) and 0.5; \( b = 20; c = 0.1 \). (b) \( a = 0.1, 0.3, \) and 0.5; \( b = 0.1; c = 0. \) (c) \( a = 0.1, 0.3, \) and 0.5; \( b = 100; c = 0. \) (d) \( a = -0.1, -0.3, \) and \(-0.5; b = 0.1; c = 0.5. \)]
CHARACTERIZATION OF SYMMETRIC PARTICLES

The length of line segment \( \overline{OB} \) is therefore

\[
\overline{OB} = \frac{\overline{OA}}{\cos((\pi/m) - \theta)} = \frac{c \cos(\pi/m)}{\cos((\pi/m) - \theta)}
\]

and the difference between \( \overline{OB} \) and the radius \( c \) is

\[
\overline{OB} - c = c \left\{ \frac{\cos(\pi/m)}{\cos((\pi/m) - \theta)} - 1 \right\}.
\]

Equation [9] is the amount to be subtracted from the circle in order to produce the polygon. This is exactly the amount that should be approximated by the \( a \) term in Eq. [1]. In order to achieve a very close approximation, the \( a \) term should be made to generate this value as closely as possible for all \( \theta \). Clearly we have to let \( m = 2n \) if Eq. [1] is to be used. In order to determine the optimum value of \( a \), we note that the wave height at \( \theta = \pi/m = \pi/2n \) generated by Eq. [1] is a maximum (i.e., the amplitude):

\[
a|\sin^2(n\theta)| = a|\sin^2(\pi/2)| = a
\]

at \( \theta = \pi/2n \),

which, in the most ideal situation, should be equal to the right-hand side of Eq. [9], i.e.,

\[
a = c \left\{ \frac{\cos(\pi/2n)}{\cos((\pi/2n) - (\pi/2n)))} - 1 \right\}
\]

\[
= c \left[ \cos\left( \frac{\pi}{2n} \right) - 1 \right]
\]

or

\[
\frac{a}{c} = \cos\left( \frac{\pi}{2n} \right) - 1.
\]

As we see in Fig. 3a, some shapes generated by Eq. [1] with appropriate values of the parameters resemble exact polygons. In this section we attempt to derive formulas for determining the optimum values of the parameters for simulating exact polygons.

Figure 4 shows a sector of an exact polygon which is circumscribed by the circle with center at \( O \) and radius \( c \). If the polygon is \( m \)-sided, then the angle \( \angle COA \) is \( \pi/m \). The length of the line segment \( \overline{OA} \) is

\[
\overline{OA} = c \cos(\pi/m).
\]
TABLE I

<table>
<thead>
<tr>
<th>n</th>
<th>a/c</th>
<th>b</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.5</td>
<td>-0.500</td>
<td>0.292</td>
</tr>
<tr>
<td>2</td>
<td>-0.2929</td>
<td>0.355</td>
</tr>
<tr>
<td>2.5</td>
<td>-0.1910</td>
<td>0.382</td>
</tr>
<tr>
<td>3</td>
<td>-0.1339</td>
<td>0.397</td>
</tr>
<tr>
<td>3.5</td>
<td>-0.0990</td>
<td>0.406</td>
</tr>
<tr>
<td>4</td>
<td>-0.0761</td>
<td>0.412</td>
</tr>
<tr>
<td>4.5</td>
<td>-0.0603</td>
<td>0.416</td>
</tr>
<tr>
<td>5</td>
<td>-0.0489</td>
<td>0.418</td>
</tr>
<tr>
<td>5.5</td>
<td>-0.0405</td>
<td>0.421</td>
</tr>
<tr>
<td>6</td>
<td>-0.0341</td>
<td>0.422</td>
</tr>
<tr>
<td>6.5</td>
<td>-0.0291</td>
<td>0.423</td>
</tr>
<tr>
<td>7</td>
<td>-0.0251</td>
<td>0.424</td>
</tr>
<tr>
<td>7.5</td>
<td>-0.0219</td>
<td>0.425</td>
</tr>
<tr>
<td>8</td>
<td>-0.0192</td>
<td>0.426</td>
</tr>
<tr>
<td>8.5</td>
<td>-0.0170</td>
<td>0.427</td>
</tr>
<tr>
<td>9</td>
<td>-0.0152</td>
<td>0.428</td>
</tr>
<tr>
<td>9.5</td>
<td>-0.0136</td>
<td>0.428</td>
</tr>
<tr>
<td>10</td>
<td>-0.0123</td>
<td>0.428</td>
</tr>
</tbody>
</table>

Thus for given values of c and n, the optimum a value can be calculated from Eq. [12]. To find the optimum value of b, we put Eq. [11] in the a term of Eq. [1] and require that the resultant a term should approximate Eq. [9] for all $\theta$, i.e.,

$$c \left[ \cos \left( \frac{\pi}{2n} \right) - 1 \right] [\sin^2(n\theta)]^b$$

$$\approx c \left[ \frac{\cos(\pi/(2n))}{\cos((\pi/(2n))-\theta)} - 1 \right]$$

or

$$[\sin^2(n\theta)]^b$$

$$\approx \left[ \frac{\cos(\pi/(2n))/\cos((\pi/(2n))) - 1}{\cos(\pi/(2n)) - 1} \right]$$

5. NEGATIVE WIDTH PARAMETER $b$

So far we have assumed that the values of $b$ are positive. However, $b$ can also be assigned negative values, in which case the generated shapes no longer look like any particles in the usual sense. This is because for negative $b$ values, Eq. [1] has singularities at $\theta = k\pi/n$ where $k = 0, 1, 2, 3, \ldots, 2n$. Consequently the magnitude of the a term at any one of these points is infinite. Clearly $a$ should not be assigned negative values when $b$ is negative; otherwise a negative infinity value for $r$ will result. In addition, the values of $b$ should not be set to a very large value to prevent the occurrence of a very large $a$ term.

Figure 6 shows an example with $n = 2$. The shape looks like two perpendicular long fibers
with particles accumulated mainly in the intersection. Changing the value of $n$ will change the number of “fibers” while $a$, $b$, and $c$ determine the size and shape of the center block. It may be possible to use these parameters to characterize the clogging of filters. But no further detail will be explored in this paper.

6. METHODS OF FITTING

We now discuss the inverse problem of the previous discussions, namely, the determination of the values of the parameters in Eq. [1] for actual particle samples. For a large quantity of samples it is necessary to develop some computerized video techniques to carry out the fitting, or at least some semiautomatic procedures such as that carried out by Wang and Greenwald (8) for a sample of 622 hail particles. For a small number of particles, however, it is possible to manually fit the particle shape and size. This is briefly discussed in the following.

Before the fitting it is necessary to determine whether a positive or negative value of the amplitude parameter $a$ is to be used. Although sometimes either case can be chosen, it is most consistent to use positive $a$ when the radius of curvature at the tip of a branch is positive (i.e., the center of curvature lies inside the branch; see, e.g., Fig. 1a). On the other hand, when the curvature at the tip is negative (see, e.g., Fig. 2d), then a negative amplitude parameter $a$ is used.

Figure 7 shows a branch of the supposed sample particle. To fit such a particle by Eq. [1] we first determine $n$ which is one-half of the number of sides or branches of this particle. We then determine the center parameter $c$ and the amplitude parameter $a$. From Fig. 7 it is easy to see that in order to fit Eq. [1],

\[ c_1 = a(1/2)^b + c \]  \[ a \]

and

\[ c_2 = a + c, \]  \[ a \]
where \( c_1 \) and \( c_2 \) are the radial lengths at \( \theta = \pi/4n \) and \( \theta = \pi/2n \), respectively. From Eqs. [15] and [16] we immediately have

\[
b = \ln\left(\frac{c_2 - c}{(c_1 - c)}\right)/\ln 2. \tag{17}
\]

The above formulas are applicable to both positive and negative \( a \) cases. The only difference is that when \( a \) is positive, \( c \) is the radius of the center disk. When \( a \) is negative, \( c \) is the length from the center to the tip of the branch. In this manner the parameters \( a, b, c, \) and \( n \) can be determined.

7. SIMULATED SAMPLES

At present we do not have an actual sample of particles for analysis. To illustrate how Eq. [1] can be used to characterize an actual sample we use a simulated sample. Figure 8 shows such a sample. The shapes here are obviously far from spherical. The particles can be generated by Eq. [1] using \( n = 0.5 \). The distributions of the parameters of \( a, b, \) and \( c \) are shown in Figs. 9, 10, and 11, respectively. If the value of \( n \) changes, the shapes will change dramatically. It is felt that the shape-size dis-
FIG. 9. The $a$ distribution for the sample in Fig. 8.

The distributions displayed here could have happened in an actual particle sample.

8. CONCLUSIONS

We have shown that Eq. [1] can generate various polygonally symmetric shapes by varying the parameters $a$, $b$, $c$, and $n$. The effect of each parameter was discussed and examples were demonstrated. It is felt that the basic two-dimensional shapes of many particles can be represented by this expression. For an ensemble of particles whose shapes can be generated by Eq. [1], the distributions of the four parameters will serve to characterize their shapes and sizes.

FIG. 10. The $b$ distribution for the sample in Fig. 8.
The advantage of this characterization technique is that the mathematics involved is very simple; all mathematical formulas are analytical which makes the calculations of various geometrical quantities extremely easy. The interpretations of the distributions of various parameters are physically explicit and easy to understand. It is felt that whenever this technique can be applied it is simpler than other more complicated methods such as fractals or orthogonal functions (see, e.g., (9, 10)). The latter two techniques are useful in characterizing very complicated shapes. On the other hand, the technique also gives more information than do the conventional methods of size estimate or aspect ratios.

In addition to the above advantage, the present method is very convenient in specifying the boundary conditions for analytical and numerical modeling purposes. For example, in order to compute the physical properties (e.g., thermal, diffusional, or scattering) of a hexagon numerically, it would be necessary to specify first the conditions at each point on the surface of the hexagon. For an accurate account of these conditions in a numerical scheme, a large number of points would be required. This could be very cumbersome, especially when values not on the grid are needed, for then some interpolation schemes are necessary. However, if we use Eq. [1] with the parameters given in Table I, we can gen-

$$b = 1 \quad c = 0.2$$
$$n = 3$$

$$n = 2.5$$

$$n = 2$$

$$n = 1.5$$

$$n = 1$$

$$n = 0.5$$

$$a = 0.05$$
$$a = 0.1$$
$$a = 0.15$$

FIG. 12. Shapes generated by Eq. [18] with $a = 0.05$, 0.1, and 0.15; $b = 1$; $c = 0.2$. 

Journal of Colloid and Interface Science, Vol. 117, No. 1, May 1987
erate an almost exact hexagon and the boundary conditions can be easily specified by using Eq. [1].

It is also possible to produce some "surface roughness" by modifying Eq. [1]. This is done by observing that the surface irregularities are short waves (i.e., higher frequencies) superimposed on the basic wave patterns. Thus by adding a function that generates these short waves, a shape with some surface roughness can be generated. Figure 12 shows one example which is generated by the following formula:

$$r = a[\sin^2(n\theta)]^b + c + (a/3)[\sin^2(10n\theta)].$$  \[18\]

The assignment of the amplitude parameter is quite arbitrary; it merely serves to show the possibility of adding short wave patterns. The systematic implementation of this should await more detailed investigations.

ACKNOWLEDGMENTS

I thank Eva Singer and Mary Sternitzky for carefully typing the manuscript. I benefitted from many helpful discussions with Ken Beard, Harry Oches, and K. H. Leong. This work is partially supported by NSF Grant ATM-8317602 to the University of Wisconsin, Madison and Graduate Research Fund 170274 of the University of Wisconsin, Madison.

REFERENCES