Short Communication

A Simple Approximate Formula for the Aspect Ratio of Oblate Particles

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Abstract

A simple approximative formula is derived, which can be used to quantify the shape of oblate particles or an average shape of the corresponding particle system, when the results of sedimentation analysis (Stokes equivalent diameters) are known and results from either microscopic image analysis (assuming stable orientation, i.e., with the plane perpendicular to the direction of observation) or laser diffraction (assuming random orientation) are available for the same sample. In the latter case Cauchy's stereological theorem is applied to account for random orientation. Furthermore, it is shown that for sufficiently large aspect ratios, this formula is very close to the well-known Jennings-Parslow relation and can replace this more complicated expression in many practical cases, e.g., in the routine characterization of ceramic raw materials (kaolins and oxide or non-oxide platelet powders).

Keywords: aspect ratio, laser diffraction, oblate particles, particle size and shape, sedimentation analysis

It is well known that non-spherical particle shape, in particular strong anisometry, is the main reason for the differences in particle sizing results using different analysis methods [1–6], since only for a sphere the equivalent diameter, defined differently for each method, reduces to a true sphere diameter, whereas for all other shapes it is only a relative size measure. On the other hand, the characteristic differences between the results obtained by different sizing techniques, when available, can be exploited to extract shape information relevant to the particle system measured [7–9]. However, for this purpose, it is necessary to propose an idealized model to define the shape measure. In the case of oblate particles, the simplest model shapes are the circular disk, i.e., flat cylinder with circular cross-section or the oblate spheroid, i.e., rotational ellipsoid. For both models, shape can be uniquely defined via a single number, the aspect ratio. It is understood, of course, that in practice the approximation of the real particle shape by a rotationally symmetrical model is an idealization in itself, which may be more or less realistic, Figure 1. Notwithstanding this

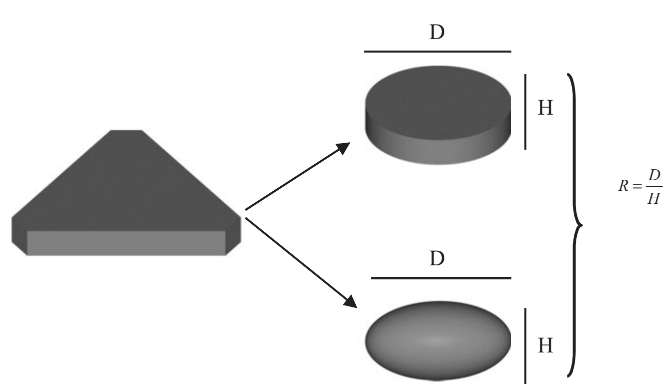

Fig. 1: Two possible model shapes (right top – disk, right bottom – oblate spheroid) approximating the real-shape platelet (left).

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shortcoming, it is in many cases the only feasible choice for routine shape characterization.

In this paper, a simple formula is derived, which enables an average aspect ratio of a particle system related to the median size to be calculated, when the particles are of oblate shape with a sufficiently high degree of anisometry. Due to its simplicity, the formula is useful for routine shape characterization. In order to apply this formula in practice, the user must have the results (measured distribution curves) from at least two types of size analyses: either sedimentation and image analysis with particles in a stable orientation, i.e., with their equatorial plane perpendicular to the direction of observation or sedimentation analysis and laser diffraction where random orientation can usually be assumed. From the aforementioned facts, it is clear that knowledge of the Stokes diameter from sedimentation analysis is the key to this method of shape determination.

Sedimentation data are usually evaluated via the classical Stokes relation:

$$D_S = \sqrt{\frac{18\,\eta\, v}{(\rho_S - \rho_L)\, g}}, \tag{1}$$

where η is the viscosity coefficient of the pure liquid medium without particles, v is the steady-state velocity, ρ_S is the density of the particles, ρ_L is the density of the liquid and g is the gravitational acceleration. The implicit assumptions adopted to derive this relation from the force balance (or the momentum balance) are well known [10,11] and may be verified for each case in question, except for the assumption of spherical particle shape, which is principally not verifiable by sedimentation alone and is responsible for the numerical factor $\sqrt{18}$ in Eq. (1). Therefore, the resulting D_S value (the so-called Stokes diameter or sedimentation diameter) is an equivalent size measure defined via Eq. (1), and in general does not correspond to any specific geometric feature of the particle (except in the very special case of spheres).

It is possible, of course, to derive a relation completely analogous to the classical Stokes relation for any well-defined particle shape, for which the resistance force term, F_R, is known. This is the case for spheroids (both prolate and oblate), where one can use the classical Oberbeck formulae [10]. In particular, in the case of infintely thin oblate spheroids (platelets or disks with a diameter D), this results in the very simple expression, Eq. (2):

$$F_R = 6\,\eta\, v D\,, \tag{2}$$

which represents an average value of the resistance force, taking into account all possible orientations of the oblate spheroidal particle (platelet) relative to the streaming medium surrounding it, i.e., averaged over all solid angles [10]. It should be noted that the classical Stokes expression for spheres is $F_R = 3\,\pi\,\eta\, v D_S$, while the two corresponding expressions for platelets settling in the normal and parallel direction are $F_R = 8\,\eta\, v\, D$ and $F_R = 16/3\,\eta\, v\, D$, respectively [11]. Eq. (2) can be used in the force balance $F_B - F_G + F_R = 0$, together with the general spheroid expressions for the lift force (buoyancy force), F_B, and the gravitational force, F_G:

$$F_B = \frac{\pi}{6}\frac{D^3}{R}\rho_L\, g, \tag{3a}$$

$$F_G = \frac{\pi}{6}\frac{D^3}{R}\rho_S\, g. \tag{3b}$$

In these expressions, R is the aspect ratio of the spheroids defined as the ratio of the large and the short (half-) axis, i.e., for platelets the equivalent circular disk diameter divided by the disk thickness. As a consequence, the resulting modified Stokes relation is given by:

$$D_M = \sqrt{\frac{36\,R}{\pi}}\sqrt{\frac{\eta\, v}{(\rho_S - \rho_L)\, g}}, \tag{4}$$

where D_M is the equatorial spheroid diameter, i.e., in practice, the equivalent circular disk diameter in the case of thin platelets with an irregular outline, corresponds to the projected area diameter, which can be directly measured via image analysis. In principle, this relation could be used to extract D_M values when the average aspect ratio can be defined for the system in question and is known a priori. On the other hand, when the D_M values are accessible from an independent measurement, e.g., from microscopic image analysis when the platelets are in a stable position, i.e., lying on the sample holder, it is possible to extract the aspect ratio from the relation:

$$R = \frac{\pi}{2}\left(\frac{D_M}{D_S}\right)^2, \tag{5}$$

which can easily be derived from the fact that $\sqrt{18}\cdot D_M = \sqrt{36/\pi}\cdot D_S$, i.e., by comparing Eqs. (1) and (4). Moreover, if the platelet orientation is random (which is a possible scenario, e.g., in laser diffraction), the aspect ratio can also be extracted, since the average projected area of randomly oriented convex particles is known to be one quarter of the surface areas of these particles from Cauchy's stereological theorem. In other words, when the laser diffraction diameter, D_L, is measured for particles in random orientation, one obtains Eq. (6):

$$R = \pi \left(\frac{D_L}{D_S}\right)^2, \tag{6}$$

which follows directly by application of the Cauchy theorem, which in the case of thin platelets leads to the conclusion that $D_M = \sqrt{2} \cdot D_L$. To elucidate the approximative status of this simple relation, Eq. (6), it is instructive to consider the exact analytical solution given for the spheroid problem by Jennings and Parslow [12]. In the current notation, the Jennings-Parslow solution can be written as:

$$\frac{D_S}{D_L} = \sqrt{\frac{2R \ \arctan\sqrt{(R^2-1)}}{R\sqrt{(R^2-1)} + \ln\left[R + \sqrt{(R^2-1)}\right]}}. \tag{7}$$

Since for $R \to \infty$, one obtains $\sqrt{(R^2-1)} \approx R$, i.e.,

$$\frac{D_S}{D_L} = \sqrt{\frac{2R \ \arctan R}{R^2 + \ln 2R}}, \tag{8}$$

and further, since for $R \to \infty$ one obtains $\arctan R \approx \pi/2$ and the term $\ln 2R$ can be neglected with respect to R^2, Eq. (6) is regained. In other words, Eq. (6) represents an approximation of the Jennings-Parslow relation, Eq. (7) for the case of thin spheroids, i.e., platelets with a large aspect ratio. In contrast to the cumbersome expression in Eq. (7), which cannot be analytically inverted, Eq. (6) is a useful formula for calculation of the aspect ratio and may be routinely used for the shape characterization of ceramic raw materials consisting of sufficiently thin platelets.

In addition to its inherent simplicity, a further evident advantage of the derivation of Eqs. (5) and (6), which are to be used in the case of perpendicular or random particle orientation, respectively, is the possibility of modifying them according to available specific information concerning particle shape. For example, when it is known a priori that the real particle shape is better represented by a disk model than by a spheroid model, Eqs. (3a) and (3b) would simply have to be modified by inserting the appropriate relations for disks to give Eqs. (3c) and (3d):

$$F_B = \frac{\pi}{4}\frac{D^3}{R}\rho_L g, \tag{3c}$$

$$F_G = \frac{\pi}{4}\frac{D^3}{R}\rho_S g. \tag{3d}$$

and the resulting approximate formula for the aspect ratio calculation would be:

$$R = \frac{3\pi}{4}\left(\frac{D_M}{D_S}\right)^2, \tag{9}$$

$$R = \frac{3\pi}{2}\left(\frac{D_L}{D_S}\right)^2, \tag{10}$$

for the case of perpendicular and random platelet orientation, respectively. Eq. (9) has been previously applied by the present authors to extract shape information and to compare the degree of anisometry of different kaolin types and other powder materials with oblate particle shape [7–9].

It should be noted that none of these relations, neither the approximate relations, Eqs. (5), (6), (9), and (10) nor the exact Jennings-Parslow solution, Eq. (7), can yield a sharp value of the aspect ratio, even in the case of a monodisperse platelet system. One reason is that the platelet orientation during settling is usually not predictable, and thus, the D_S value is only an average of a fuzzy set with a finite distribution width. The second reason is that the random orientation introduced via the Cauchy theorem makes D_L an average of a fuzzy set even for cases where the D_M value is sharp, i.e., the cumulative D_M distribution is a Heaviside step function (monodisperse system).

Of course, an advanced statistical treatment would be desirable to give a quantitative answer to the question of the type of average aspect ratio that is determined for real particle systems. This problem is highly non-trivial because of the fact that the aspect ratio does not generally need to be size invariant [13]. In combination with the aforementioned "non-sharpness", this means that the aspect ratio itself exhibits a distribution, which can be different for each size class. In other words, each size distribution is convoluted by a shape distribution. With respect to this, a word of caution might be appropriate. For practical application of Eqs. (5), (6), (9), and (10), as well as the exact solution, Eq. (7) to real particle systems (with polydisperse distributions) it is necessary to know that none of these relations can be expected to yield physically reasonable aspect ratio values based on size values obtained from the tails of the measured particle size distribution curves. Therefore, it is most reasonable to restrict attention to the central region of the distribution curves, i.e., to the median values.

In addition, it should be noted that although Eq. (6) is an excellent approximation to Eq. (7) for large aspect ratios, i.e., thin platelets, see Figure 1, it cannot be valid for small aspect ratios, i.e., particles that are close to being spherical, Figures 2 and 3. In this case Eq. (6) would erroneously predict an aspect ratio of π, and not 1 as required (since for spherical particles, the equivalent diameters D_S, D_L and D_M must all be identical to the true sphere diameter). It turns out that for particles with an aspect ratio of less than 5, the prediction via Eq. (6) is overestimated by 20 %, while for particles with aspect ratios of > 10 and > 20 the errors are below 10 % and

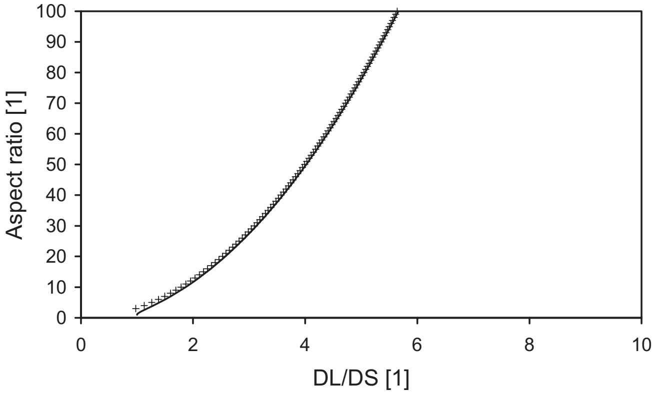

Fig. 2: Comparison of our simple approximate formula, Eq. (6) (crosses), with the exact Jennings-Parslow solution, Eq. (7) (full curve) – overview.

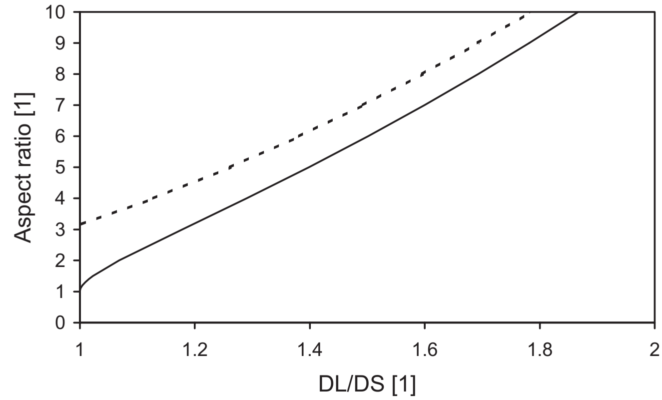

Fig. 3: Comparison of our simple approximate formula, Eq. (6) (dotted curve), with the exact Jennings-Parslow solution, Eq. (7) (full curve) – zoomed view.

5 %, respectively. For these cases, Table 1 lists the exact values resulting from the exact Jennings-Parslow solution. These values allow the users to choose their own "acceptable" errors when applying the approach presented here to oblate particles with only a small deviation from sphericity.

It should be emphasized that all relations derived in this paper are generically theoretical results, not biased by any experimental finding. Of course, the decision concerning the numerical prefactor, i.e., whether to use Eqs. (5), (6), (9), or (10) has to be based on reasonable assumptions, when the calculated values are to be physically meaningful, i.e., average, aspect ratios and not only "equivalent aspect ratios", "anisometry indices" or "shape factors" usable for relative comparison purposes only. In case of doubts, it may be useful, for example, to verify the assumption of random orientation in the measuring cell of laser diffraction instruments via image analysis. A simple method to perform this task is currently being elaborated.

Table 1: Aspect ratio as a function of the ratio D_L/D_S according to Parslow and Jennings [12].

D_L/D_S	Aspect Ratio, R
1	1
1.001	1.1
1.005	1.2
1.009	1.3
1.016	1.4
1.022	1.5
1.068	2
1.178	3
1.290	4
1.4	5
1.5	6
1.6	7
1.7	8
1.8	9
1.9	10
2.0	12
2.2	14
2.4	17
2.6	20
3.0	28

With regard to the comparison with experimental data in general, it has to be emphasized that the functional form of the relations presented in this paper is not liable to experimental verification or falsification, i.e., under the conditions explicitly stated in this paper this functional form is the only possible one. Of course, an accurate quantitatitive validation of the different numerical factors can only be made by carefully examining monodisperse and monoshaped model systems. In particular, distinguishing the numerical factors for disks from those of oblate spheroids would require artificially produced disk and spheroid systems with particles of the same aspect ratio. Such a comparison has not yet been made and to the best of our knowledge the well-defined particle systems required for this comparison, and even viable methods to produce the corresponding speroidal particles, are currently not available and unlikely to become so in the near future. In other words, at the moment there seems to be no way to experimentally validate the exact values of the numerical prefactors on the basis of synthetic model systems.

On the other hand, it should be remembered that the Parslow-Jennings relation is widely used to characterize real particle systems without the hope of similar validation, e.g., [14,15]. It should be noted that the few studies where such a comparison with independently measured aspect ratios has actually been made confirmed that the results are of the same order of magnitude and sometimes relatively close but did not exhibit numerical coincidence [16,17], so that these studies can equally well be viewed as a confirmation of the current relations, which are all within ± 50 % of the Jennings-Parslow prediction. The general success of the Jennings-Parslow relation is based on the fact that it provides a unique value of a "shape factor", which is an appropriate measure for relative comparison purposes. For kaolins, for example, the median shape factors typically exhibit values ranging from 5 to approx. 50 [14,15]. These values, of course, need not be the true (average) aspect ratios. As shown above, the extremely simple Eq. (6), with prefactor π can be used in practice as a satisfactory approximation to replace the Parslow-Jennings relation, (with more anisometric particles giving better results). In this sense, the Parslow-Jennings relation must be considered as a special case, since it has been shown in this paper that the prefactor π is obtained only under very specific assumptions.

However, even in the absence of any knowledge concerning the specific particle shape (disk or oblate spheroid) and orientation (oriented or random), Eqs. (5) and (10) with numerical prefactors 0.5π and 1.5π, respectively, provide upper and lower bounds for the true (average) aspect ratio, and thus, fulfil a task that has been completely ignored in the derivation of the Jennings-Parslow relation, i.e., taking into account the alternative possibilities of random or preferential orientation as well as the rounded or edgy nature of the platelet surface, i.e., oblate spheroids or disks, respectively. If only a relative shape measure is required, any of the Eqs. (5), (6), (9), or (10) would do just as well. However, in this case, for pragmatic reasons and reasons of compatibility with the Jennings-Parslow relation, Eq. (6) is recommended, i.e., a prefactor of π.

Nomenclature

D diameter of an oblate particle (flat cylinder or spheroid)
D_L random orientation diameter (typically from laser diffraction)
D_M equatorial spheroid or disk diameter (typically from microscopic image analysis)
D_S Stokes equivalent sphere diameter
F_B buoyancy force (lift force)
F_G gravitational force
F_R resistance force
g gravitational acceleration
H height of an oblate particle (flat cylinder or spheroid)
R aspect ratio of an oblate particle (flat cylinder or spheroid)
v steady-state settling velocity
η dynamic shear viscosity of the liquid medium
ρ_S density of the solid particle
ρ_L density of the liquid

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