

AN ESTIMATE OF ORIENTATION EFFECTS ON THE RESULTS OF SIZE DISTRIBUTION MEASUREMENTS FOR OBLATE PARTICLES

WILLI PABST, JAN MIKAČ, EVA GREGOROVÁ, JIŘÍ HAVRDA

*Department of Glass and Ceramics, Institute of Chemical Technology, Prague
Technická 5, 166 28 Prague, Czech Republic
E-mail: Willi.Pabst@vscht.cz*

Submitted January 11, 2002; accepted February 2, 2002

Keywords: Particle size distributions, Oblate particles, Laser diffraction

The influence of the orientation of oblate particles on volume-weighted particle size distributions (PSD) is demonstrated with an idealized model system. The overall estimate is based on partial "worst case" estimates found by an explicit calculation of selected non-random orientations for disk-shaped particles with an aspect ratio of 10 and a wide-range PSD. According to the simulation results the D_{10} , D_{50} (median) and D_{90} values for particle orientations of 60° , 45° , 30° and 0° deviate by less than 17 % from those of the 90° orientation (corresponding to projections normal to the disk plane), whereby the maximum deviation occurs for orientations close to 30° . For quasi-random orientation the deviation is even smaller (approx. 3-7 %). Thus it is shown that, in contrast to widespread belief, the effect of particle orientation on the resulting volume-weighted PSD is for oblate particles small enough to be completely smeared out for purely statistical reasons to within typical errors of measurement of the usual sizing methods.

INTRODUCTION

It is generally assumed that the orientation of anisometric particles has an influence on the particle size distribution measured by optical methods [1]. This is in principle true [2, 3, 4]. Actually, some recently developed methods try to exploit just this effect for particle shape characterization [5]. However, a general answer to the question how and to what extent the particle size distribution (PSD) is influenced by particle orientation in the case of anisometric particles can probably not be given. Although there are exceptional cases where the physical situation is very clear (e.g. in static microscopic image analysis), in general a thorough analysis is needed for each individual case, taking into account the measurement principle used for sizing (including the theory used for the evaluation of recorded data, e.g. Mie theory or Fraunhofer theory in laser diffraction), specific instrumental conditions (e.g. the photodetector geometry and the hydrodynamic situation - whether laminar or turbulent - in the flow-through cell in laser diffraction instruments, possibly in dependence of measurement parameters such as pump speed), the material characteristics (prolate or oblate shape, Brownian or non-Brownian size) and possibly other parameters (e.g. enhanced rotational diffusion of Brownian particles due to temperature changes). Given only the relatively simple case of a non-Brownian spheroid in isothermal laminar flow the question of whether, and if yes in what direction and after what time, the particle orients itself with respect to the flow is highly nontrivial and needs careful analysis, based on Jeffery's 1922 paper [6]. But also from a statistical point of view, the problem is far from trivial,

since for a strict analysis the effect of particle orientation on a PSD would have to be described by orientational distribution functions interacting with size distribution functions.

The aim of the present contribution is a much more modest one: Without strict limitation to a special sizing method, but confining ourselves to those methods where size information is inferred, directly or indirectly, from a projectional view of the particles without using a unique substitute diameter (e.g. the projected area diameter in image analysis), we want to present a rough estimate of how the measured PSD will be influenced under the assumption of more or less extreme particle orientations from a purely statistical point of view. More than that, we confine the presentation to certain model particles (oblate disks with a prescribed aspect ratio of 10) and an appropriately selected symmetric discrete model PSD (given in the so-called "q3" representation, i.e. in the form of a volume-weighted "frequency" histogram) for reasons of simplicity and reference. This does not mean, however, that the results are without concern for realistic systems. On the contrary, the simple argumentation presented in this paper (which is based largely on intuitive arguments), is to provide a kind of "worst case" estimate for the influence of the orientation of disk-shaped particles on measured PSD curves. The disk model should be an acceptable approximation of platey particles for most practical purposes. The aspect ratio of 10 used here is a pragmatic choice of course. The model PSD investigated is chosen sufficiently wide (comprising particles with equivalent diameters ranging from 1 to 100 μm) to be rather realistic.

The main question to be answered is: How large is approximately, for the model system investigated, the influence of particle orientation on a measured PSD? In other words, and maybe more precisely: What is the maximal difference of the PSD in terms of equivalent disk diameters for extreme non-random particle orientations?

No attempt is made to solve the problem strictly, neither to find the extreme aspect ratio for which this difference (i.e. the orientational effect on the PSD) is maximal, although it is clear that such a "critical" aspect ratio must exist (since for an infinite aspect ratio, i.e. infinitely thin disks, and for an aspect ratio of 1, i.e. for isometric particles, the PSD is not influenced by particle orientation), nor to find the extreme intermediate orientation for which this difference is maximal, although also in this case it will turn out that such a "critical" orientation must exist (since the PSD for 100 % frontal orientation is very close to that for 100 % lateral orientation, as will be shown below).

Notwithstanding the great practical importance of this problem, e.g. for the extraction of shape information from particle size measurements [7,8,9,10], to the authors' knowledge no general solution of the aforementioned problem is available in the literature so far. Therefore we present this rather clumpy demonstration of a special case to a wider audience of readers, hopefully as an impetus to a more stringent formulation and more general solution of the problem in the future. It will be shown that for the system investigated (and probably for most realistic systems with oblate particles) the PSD (more precisely, the volume-weighted PSD, since this is what is usually meant by the practitioner) is substantially uninfluenced by particle orientation, in contrast to widespread belief. Thus it will be shown that, to within typical errors of measurement (naturally depending on the sizing method), the differences possibly caused by particle orientation are largely smeared out for purely statistical reasons in a volume-weighted PSD. For measuring principles and statistical aspects of particle sizing the reader should refer to standard references, e.g. [1] and [11].

SIMULATION MODEL AND METHOD

Model particles and model PSD

Disk-shaped particles of expressedly oblate shape with an aspect ratio (i.e. diameter-to-height ratio) of 10 have been chosen as model particles for this study. The shape of the particles is assumed to be scale-invariant, i.e. whatever the absolute size the particles are to remain disk-shaped with an aspect ratio of 10.

The model PSD is given in the form of a volume-weighted "frequency histogram" (i.e. a "q3" distribution) with relative volumes of 1, 3, 7, 15, 7, 3, 1 for particles with equivalent diameters of 1, 2, 5, 10, 20, 50, 100 μm , respectively (see figure 1). For reasons of simplicity this model PSD has been chosen symmetric and discrete.

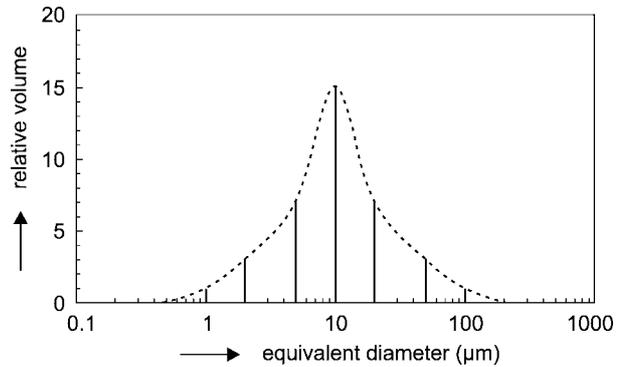


Figure 1. Volume-weighted model PSD („q3“ histogram) corresponding to a relative volume of 1, 3, 7, 15, 7, 3, 1 for particles with equivalent diameters 1, 2, 5, 10, 20, 50 and 100 μm , respectively.

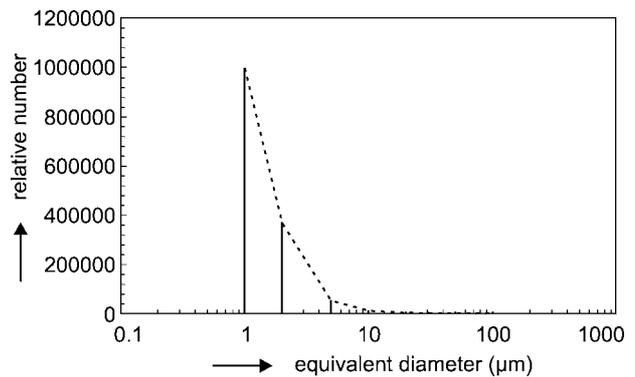


Figure 2. Number-weighted model PSD („q0“ histogram) corresponding to a relative volume of 1, 3, 7, 15, 7, 3, 1 for particles with equivalent diameters 1, 2, 5, 10, 20, 50 and 100 μm , respectively.

This PSD can be imagined as being measured in the case of spherical particles or, equivalently, for the case that all disk-shaped particles are oriented exactly with their plane normals parallel to the direction of observation. Thus in the above setting the notion equivalent diameter has to be understood as the disk diameter proper.

When this volume-weighted PSD is transformed into a number-weighted PSD (i.e. a discrete "q0" distribution) one obtains the picture shown on figure 2, cf. the values in table 1.

Table 1. Model PSD ("q3", i.e. volume-weighted) and the same transformed into a number-weighted ("q0") PSD (equivalent diameter corresponding to the disk diameter proper).

equivalent diameter (μm)	relative volume	relative number
1	1	1000000
2	3	375000
5	7	56000
10	15	15000
20	7	875
50	3	24
100	1	1

Note that for the above transformation no assumption on particle shape is necessary. The transformation is valid for spheres as well as for all types of oblate particles with circular projection (e.g. cylinders or spheroids) as long as they are uniquely oriented with their plane normals parallel to the direction of observation. It should be kept in mind that in the original volume-weighted PSD one particle of diameter 100 μm has the same statistical weight as one million particles with diameter 1 μm . That means that only a few particles determine the course of the PSD in the large-size region, compared to the large amount of particles in the small-size region.

The simulation method

Figure 3 shows, for the model particles chosen, a schematic view of five special particle orientations with respect to the direction of observation (say, the laser beam direction in a LALLS measurement): 0° (plane normal perpendicular), 30°, 45°, 60° and 90° (plane normal parallel).

In the 0° orientation the disk-shaped particle appears to the observer simply as a rectangle with a side ratio of 1:10. Thus an automatic detecting device in which directional information is lost (say, a circular or half-circular photodetector in a LALLS measurement)

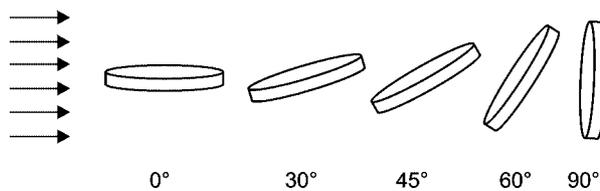


Figure 3. Schematic view of the disk-shaped model particles in five special orientations with respect to the direction of observation.

would "see" (although not directly, but via Fourier transformation encoding) ten times more small particles (of diameter $D/10$) than large particles (of diameter D), irrespective of the absolute particle size (diameter). In a model calculation these erroneous additional counts of ten small particles in connection with the one large particle can be accounted for in a straightforward way by adding ten times the number of particles with diameter D to those of diameter $D/10$ in the number-weighted PSD, cf. the third column in table 2.

While the above assumptions for the case of 0° orientation are quite plausible, and the case of 90° orientation is obviously trivial, intermediate orientations cannot be treated in an elementary way without adopting rough approximations. Considering the substitute minimum diameters in table 3 (calculated by adding the projection of the diameter and that of the height in the respective orientation) it is evident that the minimum dimension for a particle with diameter D in 30° orientation is close to $D/2$, while that for a particle in 60° orientation is close to D itself and the 45° case lies in between. In order to preserve the original discrete abscissa values of the model PSD we adopt the following "worst case" estimate: For the 60° case we increase the weight (in the "q0" PSD) of the maximum diameter, i.e. instead of assigning e.g. one particle to 10 mm and one to 9.160 μm (which appears to be a better approxi-

Table 2. The model PSD transformed into number-weighted PSDs under the assumption that all particles are viewed under angles of 0°, 30°, 45°, 60° and 90°, respectively.

$D/\sin \alpha$ (μm)	$H/\cos \alpha$ (μm)	relative number for 0°	relative number for 30°	relative number for 45°	relative number for 60°	relative number for 90°
0.1	0.01	1000000	---	---	---	---
0.2	0.02	3750000	---	---	---	---
0.5	0.05	560000	2000000	1000000	500000	---
1	0.1	1150000	1750000	1375000	1187500	1000000
2	0.2	383750	487000	431000	403000	375000
5	0.5	56240	86000	71000	63500	56000
10	1	15010	16750	15875	15437.5	15000
20	2	875	923	899	887	875
50	5	24	26	25	24.5	24
100	10	1	1	1	1	1

Table 3. Substitute minimum diameters (μm) for particles viewed in certain orientations with respect to the direction of observation.

$D/\sin \alpha$ (μm)	$H/\cos \alpha$ (μm)	30° ($0.5D+0.866H$)	45° ($0.7071D+0.0707H$)	60° ($0.866D+0.5H$)
1	0.1	0.5866	0.7778	0.9160
2	0.2	1.173	1.556	1.832
5	0.5	2.933	3.889	4.580
10	1	5.866	7.778	9.160
20	2	11.73	15.56	18.32
50	5	29.33	38.89	45.80
100	10	58.66	77.78	91.60

mation to reality, but causes problems with matching to the original abscissa values or size classes) we assign two particles to 10 μm and one particle to 5 μm (the original size classes), cf. table 2. The latter leads doubtlessly to a more serious distortion of the PSD than the first and can thus be called a "worst case" estimate. For the case of 30° orientation we increase the weight of the substitute minimum diameter (by adding twice the number of a certain size class to the next lower size class, cf. table 2), and for the case of 45° orientation we add the number of a certain size class to the next lower size class, cf. table 2.

In order to facilitate the comparison of the results in usual representation the number-weighted ("q0") PSDs were retransformed to volume-weighted ("q3") PSDs and finally integrated by summing up the individual columns of the frequency histograms. After certain averaging procedures (necessary to eliminate artefacts resulting from the discrete nature of the model PSD) the resulting volume-weighted cumulative ("Q3") undersize PSDs were represented as smooth curves using spline fitting. Characteristic values D_{10} , D_{50} (median) and D_{90} were calculated from linear interpolation of the respective cumulative undersize values. All calculations were performed on Microsoft Excel 97 spreadsheets.

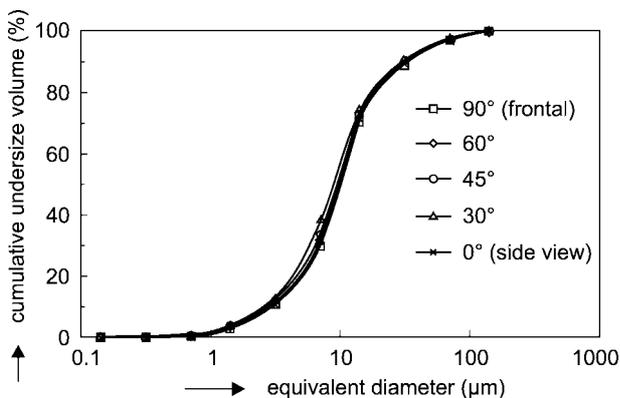


Figure 4. Calculated PSD (cumulative undersize curves in logarithmic mean scale) for the case that all particles in the system are oriented with the disk plane at angles 90° (squares), 60° (diamonds), 45° (circles), 30° (triangles) and 0° (crosses), respectively.

RESULTS

Figure 4 shows the calculated PSDs (cumulative undersize curves) for the case that all particles in the system are uniquely oriented, viz. with the disk plane at angles 90° (frontal view, i.e. with the plane normal parallel to the direction of observation), 60°, 45°, 30° and 0° (side view, i.e. with the plane normal perpendicular to the direction of observation), respectively.

In order to eliminate coarse artefacts resulting from the discrete nature of the model PSD (frequency histogram) chosen, the cumulative curves were corrected using the arithmetic mean of the logarithms of two adjacent equivalent diameters and assigning the respective cumulative percentage values to these corrected equivalent diameters (logarithmic mean scale). From the viewpoint of the cumulative PSD obtainable simply by summing up the relative volumes from the left (for such a PSD the median value e.g. is totally in error) this new, corrected PSD is shifted in the direction of increasing equivalent diameters. Table 4 lists the three characteristic values D_{10} , D_{50} (median) and D_{90} for the five PSD curves obtained by interpolation in linear scale. For reasons of comparison a "quasi-random" case has been constructed by averaging the respective values for 90°, 60°, 30° and 0° orientation. This "quasi-random" case can be considered as a rough approximation to the (practically important) random case.

Since the frequency histogram for the case of 90° orientation (i.e. observation of all disks in the direction parallel to their normals) is identical with that of spheres (note that disks observed frontally are indistin-

Table 4. Model PSD ("q3", i.e. volume-weighted) and the same transformed into a number-weighted ("q0") PSD (equivalent diameter corresponding to the disk diameter proper).

orientation	D_{10} (μm)	D_{50} (median) (μm)	D_{90} (μm)
90°	2.99	10.61	35.53
60°	2.85	10.32	33.69
45°	2.73	10.05	31.92
30°	2.59	9.28	30.73
0°	2.82	10.52	35.05
quasi-random	2.81	10.18	33.75

guishable from spheres), it is clear that the deviation of the calculated median value of 10.61 μm from the expected value of 10 μm (i.e. a median equal to the mode in our case of a symmetric frequency histogram) is an artefact resulting from the averaging algorithm and the interpolation method applied. The values D_{10} and D_{90} exhibit similar errors. Unfortunately there is no straightforward way to avoid such artefacts without affecting the discrete scale on the abscissa. One simple possibility to correct at least the median values is a rescaling of all D_{50} values with the factor $0.9425 = (10/10.61)$. The correspondingly corrected values are listed in table 6. Another possibility, which improves also the D_{10} and D_{90} values, is to apply a (discrete) transformation scheme, which is based on the arithmetic mean values between adjacent equivalent diameters but modifies them in such a way that the central region of the PSD is (artificially) calibrated with respect to the expected median value and all other equivalent diameters which are relevant in the frequency histogram result exactly as arithmetic means between the new intermediate values. Unfortunately, this discrete transformation scheme (which has been found by trial and error), although being a useful tool for the case in question here, is not generally applicable and cannot be replaced by any analytical averaging algorithm. Table 5 compares the original scale, the intermediate scale formed by the logarithmic averaging algorithm described above (arithmetic means of logarithms of adjacent equivalent diameters), arithmetic mean values of the original scale (arithmetic means of adjacent equivalent diameters) and the intermediate scale formed by the discrete transformation scheme

Table 5. Original logarithmic scale, intermediate scale formed by the logarithmic averaging algorithm (logarithmic mean scale/LM scale), arithmetic mean values of the original scale (arithmetic mean scale) and intermediate scale formed by the discrete transformation scheme (DTS scale); all values in μm .

original log scale	LM scale	arithmetic mean scale	DTS scale
0.1	0.1414	0.15	0.1
0.2	0.316	0.35	0.3
0.5	0.707	0.75	0.7
1	1.414	1.5	1.3
2	3.16	3.5	2.7
5	7.07	7.5	7.3
10	14.14	15	12.7
20	31.6	35	27.3
50	70.7	75	72.7
100	141.4	150	127.3
200	316	350	272.7
500	707	750	727.3
1000	1414	1500	1272.7

(DTS) described above, which approximates the latter and is exactly calibrated with respect to the median value.

Figure 5 shows, for the orientation 90° , the original PSD with its artificial shift to the left (this shift being an artefact resulting from the simple summing up of the discrete model PSD from the left, see above), the same PSD shifted by one discrete step (i.e. from 1 to 2 μm , from 2 to 5 μm , from 5 to 10 μm etc.) to the right, the logarithmic mean PSD (corrected according to the logarithmic averaging algorithm) and the DTS-rescaled PSD.

Both the LM-scaled PSD and the DTS-rescaled PSD lie between the original PSD (dotted in figure 5) and the shifted PSD (dashed in figure 5). The shape of the LM-scaled PSD corresponds rather closely to that of the original curves, while the DTS-rescaled PSD looks slightly distorted. Only the DTS-rescaled PSD, howev-

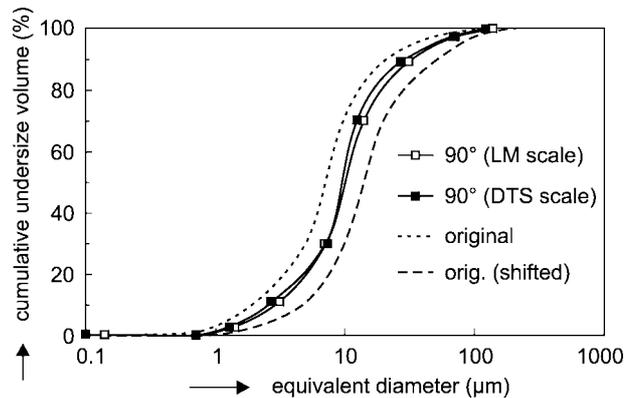


Figure 5. Cumulative undersize PSD curves for the case of 90° orientation (frontal view) using the logarithmic mean scale (hollow squares) and the DTS scale (full squares); both lie between the original PSD (dotted) with its artificial shift to the left, and the PSD shifted by one column in the model frequency histogram (dashed).

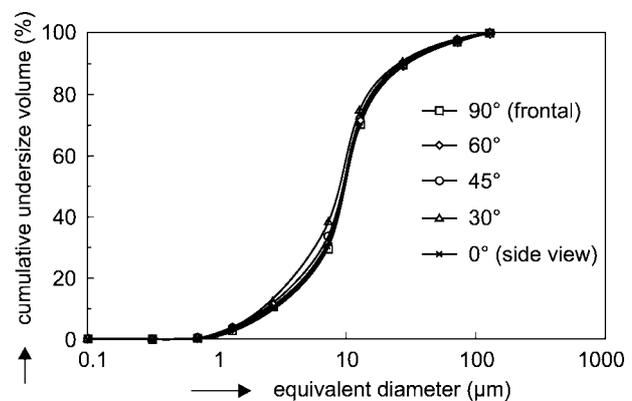


Figure 6. Calculated PSD (cumulative undersize curves in DTS scale) for the case that all particles in the system are oriented with the disk plane at angles 90° (squares), 60° (diamonds), 45° (circles), 30° (triangles) and 0° (crosses), respectively.

Table 6. Characteristic values D_{10} , D_{50} (median) and D_{90} of the DTS-rescaled PSD curves and corrected D_{50} values obtained by rescaling the D_{50} values of table 4 by the correction factor 0.9425; all values in dependence of the particle orientation (disk plane at angles 90° , 60° , 45° , 30° , 0°).

orientation	D_{10} (μm) (DTS - rescaled PSD)	D_{50} median (μm) (DTS - rescaled PSD)	D_{90} (μm) (DTS - rescaled PSD)	D_{50} median (μm) (from table 4 rescaled by the factor 0.9425)
90°	2.56	10.00	31.84	10.00
60°	2.45	9.78	29.70	9.73
45°	2.36	9.57	27.64	9.47
30°	2.24	8.99	26.55	8.75
0°	2.43	9.94	31.28	9.92
quasi-random	2.42	9.68	29.84	9.60

er, ensures that cumulative undersize and oversize PSD curves intersect exactly at an ordinate value of 50 %, as required by elementary statistics [11].

Table 6 lists the values of D_{10} , D_{50} (median) and D_{90} calculated by interpolation (in linear scale) from the DTS-rescaled cumulative undersize PSD curves (see figure 6) and, for reasons of comparison, the median values obtained via simple rescaling by the correction factor 0.9425 (see above). Note, however, that all the above considerations concerning scaling serve only to eliminate calculation artefacts resulting from the discrete (and "coarse-grained") nature of our model PSD (frequency histogram) and have nothing to do with the physical content of the simulation results. Moreover, they may well be without relevance for more realistic PSD curves, where the histogram is sufficiently "fine-grained" to be replaced by a continuous curve.

Irrespective of the rescaling procedure used, the following can be said with reference to figures 4 through 6 and tables 4 and 6: The cumulative PSD curves for different particle orientations are altogether rather close. Tables 7 and 8 show the percentual deviations of the calculated values D_{10} , D_{50} and D_{90} for the respective special orientations and the "quasi-random" case (average of 90° , 60° , 30° and 0° values) from those of the 90° case.

The calculated median (expected value $10.00 \mu\text{m}$) differs by maximally 10.1-12.5 % for either of the special orientations investigated, see tables 7 and 8. With regard to the logarithmic scale this deviation of the median value is relatively small. For D_{10} and D_{90} the

deviations from their 90° counterparts are clearly larger (12.5-16.6 %) but principally the same qualitative assessment applies. For "quasi-random" orientation the deviation of the median values is 3-4 % and for D_{10} and D_{90} only slightly larger (5-7 %). With regard to possible errors of measurement (including sampling errors) deviations of such a magnitude can be considered as small. Interestingly, the difference in the median (D_{50}) is as small as 0.6-0.8 %, i.e. practically zero, for the extreme case of 0° orientation, which means that the median of a PSD measured for the extreme case that all particles are oriented with their disk planes parallel to the direction of observation is virtually indistinguishable from that of the case where all particles are viewed frontally. The same holds true for the D_{90} value. The results indicate that the maximum deviation from the expected D_{10} , D_{50} and D_{90} values will occur for intermediate orientations (close to 30°). Concerning the individual PSD curves there is a maximum deviation at intermediate sizes on the left from the median, but the exact position of the maximum deviation is naturally a consequence of the special shape of the model PSD.

DISCUSSION

The aforementioned results show the following: For an idealized system of disk-shaped particles with an aspect ratio of 10 our calculations assuming the selected model PSD (given by a discrete "frequency" histogram, i.e. a volume-weighted PSD which appears

Table 7. Percentual deviation (%) of D_{10} , D_{50} (median) and D_{90} values (calculated from LM-scaled PSD curves) from the 90° orientation for special orientations (60° , 45° , 30° , 0°) and "quasi-random" orientation.

orientation	D_{10}	D_{50}	D_{90}
60°	-4.7	-2.7	-5.2
45°	-8.7	-5.3	-10.2
30°	-13.4	-12.5	-13.5
0°	-5.7	-0.8	-1.4
quasi-random	-6.0	-4.1	-5.0

Table 8. Percentual deviation (%) of D_{10} , D_{50} (median) and D_{90} values (calculated from DTS-rescaled PSD curves) from the 90° orientation for special orientations (60° , 45° , 30° , 0°) and "quasi-random" orientation.

orientation	D_{10}	D_{50}	D_{90}
60°	-4.3	-2.2	-6.7
45°	-7.8	-4.3	-13.2
30°	-12.5	-10.1	-16.6
0°	-5.1	-0.6	-1.8
quasi-random	-5.5	-3.2	-6.3

symmetric in the so-called "q3" representation) described above demonstrate that the cumulative under-size PSD curve is changed only rather insignificantly even in the very special case of a particular orientation of all particles in the system. Median values deviate by maximally 10-12.5 %, D_{10} and D_{90} values by maximally 12.5-16.6 % for the cases investigated. It might deserve special attention that the case of 0° orientation is closer to the case of 90° orientation (which corresponds to the equivalent sphere case) than any other intermediate orientation. Consequently, for the median values e.g. a maximum deviation from the expected value will occur at intermediate orientations (in our case close to 30°). To find the exact orientation for which this maximum deviation occurs is a straightforward task in principle, but clumpy in practice and unnecessary for our purpose, since it does not provide substantial general information in addition to that already known. In particular it is evident that the orientation for which maximum deviation occurs depends critically on the special choice of the aspect ratio.

Note that the special choice of the aspect ratio ($\psi=10$) has been made in this paper for pragmatic reasons. It should, however, not be too unrealistic. From the viewpoint of practical applications it might serve as a reasonable approximation e.g. for kaolins, some clays or tabular alumina, for which aspect ratios of this order of magnitude can well be expected (for these types of materials values of $5 \leq \psi \leq 50$ can be expected [7,8,9]). It has also to be remembered that for isometric particles ($\psi \rightarrow 1$) orientation effects are negligible whereas, on the other hand, for extremely anisometric disks ($\psi \rightarrow \infty$), although orientation effects might be more probable, the volume-weighted PSD is affected only negligibly by the thickness of the disks. That means, also with respect to the aspect ratio there is an extremum for which the PSD is most critically influenced by possible orientation effects.

Also the model PSD (frequency histogram) chosen is idealized (e.g. symmetric). Its width (comprising two orders of magnitude) corresponds, however, to a typical PSD measured by LALLS for realistic particle systems. The behavior of other model PSDs is currently being investigated.

As mentioned before, throughout this study we have assumed that all particles, without exception and whatever be their size, are orientated in a particular way. This assumption is far from realistic and unnecessarily strong. In practice, only two cases of orientation are of major relevance for particle sizing, viz. the case of 90° orientation (corresponding to orientation of the particles in the flow direction, say in the optical cell of a LALLS sizer, with the plane parallel to the shear planes of flow, i.e. perpendicular to the laser beam direction) and the case of statistical (random) orientation. Tables 7 and 8 compare, for LM-scaled and DTS-rescaled PSD curves, respectively, the percentual deviation from the expected values (corresponding to the case of 90° orientation) for the special orientations 60° , 45° , 30° and 0° and for the

case of "quasi-random" orientation obtained by taking the average of the 90° , 60° , 30° and 0° orientations. The median values are $10.61 \mu\text{m}$ (90°) and $10.18 \mu\text{m}$ ("quasi-random") and $10.00 \mu\text{m}$ (90°) and $9.68 \mu\text{m}$ ("quasi-random") for the LM-scaled and DTS-rescaled PSD, respectively. Thus the D_{50} (median) values for "quasi-random" orientation differ from those of the 90° orientation by only approx. 3-4 %. For the D_{10} and D_{90} values the deviation is slightly larger (approx. 5-7 %), but still small enough to be negligible with respect to the usual precision of measurement results. Since in reality no system will exhibit absolute (100 %) particle orientation the differences are further smeared out, when realistic measurements are concerned.

For practical work in particle sizing the results of this study can be summarized in the qualitative statement that a volume weighted PSD is only insignificantly affected by particle orientation when the particles are disk-shaped with an aspect ratio around 10. The possible error in the median value does certainly not exceed a few percent, which is practically negligible with respect to the errors of measurement of most practical sizing methods and commercial instruments exploiting the aforementioned principles.

With some improvements of technical nature and possible automatization the simulation method proposed in this paper is applicable to arbitrary PSDs and can be used to test the orientation dependence of concrete measuring results when reasonable a priori assumptions can be made concerning particle shape. It has only to be ensured that the real measurement is performed in sufficiently dilute systems in order to effectively exclude overlapping particle projections.

We like to stress, however, that neither the method applied in this study, nor any of our results, can be generalized to particles of prolate shape (e.g. needles or fibres). On the contrary, in this latter case it seems that particle orientation effects caused under certain circumstances by shear flow in the measuring cell of a laser diffractometer can be exploited to provide shape information (the aspect ratio) directly from LALLS measurements when an appropriate (wedge-shaped) photodetector is chosen and the scattering signal (diffracted light intensity pattern) is recorded under two perpendicular orientations of the photodetector [5]. This is not possible for oblate particles.

CONCLUSION

It has been shown that the influence of particle orientation on PSD measurements, although unquestionable in principle, may under certain circumstances be without practical relevance.

Based on a straightforward stepwise simulation of PSD measurements of uniquely oriented disks (idealized model particles with an aspect ratio of 10) distributed according to a symmetric discrete frequency histogram (an idealized model PSD) the resulting PSDs

have been explicitly calculated for five different orientations (90° , 60° , 45° , 30° , 0°) and expressed in the form of cumulative undersize curves. Very similar procedures, possibly automatized, could be used to test the influence of the particle orientation effect on PSD measurement for other types of oblate particles (e.g. spheroids), for particles with another aspect ratio and for other model PSDs.

A quantitative comparison of the three characteristic values D_{10} , D_{50} (median) and D_{90} for the five cases examined reveals that the deviations are relatively small (less than 17 % for all the cases with unique orientation, highest for the 30° case).

Notwithstanding this "worst cases", viz. the extreme cases of unique orientation of all particles in the system (an unnecessarily strict and unrealistic assumption) only two cases are of major practical importance: the case of 90° orientation and the case of random orientation. The "quasi-random" case constructed in this paper (simply by averaging the results of the 90° , 60° , 30° and 0° orientation) might serve as a rough approximation of the latter. It exhibits a deviation of only approx. 3-7 %. The PSD is thus essentially insensitive to orientational effects when oblate disk-shaped particles with an aspect ratio of 10 are considered. Since the same must be true for very low aspect ratio (i.e. more or less isometric particles for which $\psi \rightarrow 1$) and very high aspect ratio (i.e. $\psi \rightarrow \infty$ corresponding, say, to thin sheets), where the difference between the PSDs also vanishes, it can be conspected that this qualitative conclusion is of rather general validity.

For practical applications this means that when no directional information is recorded in particle size measurements (e.g. in LALLS with a circular or half-circular photodetector) the median value e.g. remains almost invariant (at least with regard to the precision of measurement), irrespective of the hydrodynamic situation during measurement.

Acknowledgements:

The authors thank Dr. Christoph Berthold from the University of Tübingen (Germany) for helpful discussions on the detector geometry of laser particle sizers. Partial support of a bilateral Czech-German cooperation project by the Czech Ministry of Education, Youth and Sports (Project MŠMT No. CZE 01/012) and the German Bundesministerium für Bildung und Forschung is gratefully acknowledged.

References

- Allen T.: *Particle Size Measurement*, 5th edition. Chapman & Hall, London 1997.
- van de Hulst H.C.: *Light Scattering by Small Particles*, Wiley, New York 1957.
- Kerker M.: *The Scattering of Light and Other Electromagnetic Radiation*, Academic Press, New York 1969.
- Bohren C.F., Huffman D.R.: *Absorption and Scattering of Light by Small Particles*, Wiley, New York 1983.
- Berthold C., Klein R., Lühmann J., Nickel K.G.: *Part.Syst.Charact.* 17, 113 (2000).
- Jeffery G.B.: *Proc.Roy.Soc.London, A* 102, 161 (1922).
- Kuneš K., Pabst W., Havrda J., Gregorová E.: *British Ceramic Proceedings* 60, 129 (1999).
- Pabst W., Kuneš K., Havrda J., Gregorová E.: *J.Eur. Ceram.Soc.* 20, 1429 (2000).
- Pabst W., Kuneš K., Gregorová E., Havrda J.: *Brit. Ceram.Trans.* 100, 106 (2001).
- Pabst W., Kuneš K., Gregorová E., Havrda J.: *Key Engineering Materials* 206-213, 743 (2002).
- Herdan G.: *Small Particle Statistics*, 2nd edition. Butterworths, London 1960.

ODHAD VLIVU ORIENTACE ČÁSTIC NA VÝSLEDKY MĚŘENÍ ROZDĚLENÍ VELIKOSTÍ U ČÁSTIC DESTIČKOVÉHO TVARU

WILLI PABST, JAN MIKAČ, EVA GREGOROVÁ, JIŘÍ HAVRDA

*Ústav skla a keramiky,
Vysoká škola chemicko-technologická v Praze,
Technická 5, 166 28 Praha*

Vliv orientace destičkových částic na výsledky měření objemově váženého rozdělení velikostí částic je odhadován na základě pevně zvoleného (dostatečně širokého) diskretního rozdělení velikostí idealizovaného systému modelových částic ve tvaru plochých válců (poměr průměru k výšce 10:1). Toto diskretní rozdělení lze považovat za rozumnou aproximaci mnoha výsledků získaných na reálných soustavách. Celkový odhad je založen na parciálních odhadech, které vycházejí z nejextrémnějších (tj. nejnejpříznivějších) možností, tj. případů, kdy všechny částice mají stejnou speciální orientaci v určitém směru. Pro vybrané orientace jsou provedeny explicitní výpočty rozdělení, a tím simulovány výsledky, které by byly naměřeny v případě preferenční orientace částic. Podle výsledků simulace kvantily D_{10} , D_{50} (medián) a D_{90} vykazují pro orientace částic 60° , 45° , 30° a 0° odchylku menší než 17 % od hodnoty odpovídající orientaci částic 90° (tj. projekce ve směru kolmém k ploše destiček), přičemž maximální odchylka vyplývá pro orientaci okolo 30° . Tyto výsledky se však týkají zbytečně přísně omezujících a pro praxi téměř bezvýznamných případů, kdyby všechny částice vykazovaly jednoznačně orientaci lišící se od orientace kolmé. Daleko reálnější pro běžná zařízení k měření rozdělení velikostí částic (např. laserovou difrakcí) je situace, kdy částice jsou buď orientovány kolmo, nebo vůbec ne (tj. vykazují zcela nahodilou orientaci). V tomto případě ukazují simulační výsledky, že zmíněná odchylka je ještě menší (cca. 3-7 %). Z práce vyplývá, že - oproti rozšířenému názoru - vliv orientace částic destičkového tvaru na výsledky měření objemově vážených rozdělení velikostí částic běžnými metodami (např. laserovou difrakcí), ačkoliv principiálně vždy přítomný, je ve většině reálných případů zanedbatelně malý.