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Representation of results of particle size analysis - Part 2: Calculation of average particle sizes/diameters and moments from particle size distributions (ISO 9276-2:2014,IDT)

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Representation of results of particle size analysis —

Part 2:
Calculation of average particle sizes/diameters and moments from particle size distributions

Représentation de données obtenues par analyse granulométrique —

Partie 2: Calcul des tailles/diamètres moyens des particules et des moments à partir de distributions granulométriques

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Contents

Page

Foreword .... **iv**

Introduction .... **v**

1 Scope **1**

2 Normative references **1**

3 Definitions, symbols and abbreviated terms **1**

4 The moment-notation **3**

4.1 Definition of moments according to the moment-notation 3

4.2 Definition of mean particle sizes according to the moment-notation 4

4.3 Calculation of moments and mean particle sizes from a given size distribution 7

4.4 Variance and standard deviation of a particle size distribution 9

4.5 Calculation of moments and mean particle sizes from a lognormal distribution 9

4.6 Calculation of volume specific surface area and the Sauter mean diameter 10

5 The moment-ratio-notation **10**

5.1 Definition of moments according to the moment-ratio-notation 10

5.2 Definition of mean particle sizes according to the moment-ratio-notation 11

5.3 Calculation of mean particle sizes from a given size distribution 13

5.4 Variance and standard deviation of a particle size distribution 14

5.5 Relationships between mean particle sizes 15

5.6 Calculation of volume specific surface area and the Sauter mean diameter 16

6 Relationship between moment-notation and moment-ratio-notation **16**

7 Accuracy of calculated particle size distribution parameters **18**

Annex A (informative) **Numerical example for calculation of mean particle sizes and standard deviation from a histogram of a volume based size distribution** **19**

Annex B (informative) **Numerical example for calculation of mean particle sizes and standard deviation from a histogram of a volume based size distribution** **22**

Annex C (informative) **Accuracy of calculated particle size distribution parameters** **25**

Bibliography **27**

Foreword

ISO (the International Organization for Standardization) is a worldwide federation of national standards bodies (ISO member bodies). The work of preparing International Standards is normally carried out through ISO technical committees. Each member body interested in a subject for which a technical committee has been established has the right to be represented on that committee. International organizations, governmental and non-governmental, in liaison with ISO, also take part in the work. ISO collaborates closely with the International Electrotechnical Commission (IEC) on all matters of electrotechnical standardization.

The procedures used to develop this document and those intended for its further maintenance are described in the ISO/IEC Directives, Part 1. In particular the different approval criteria needed for the different types of ISO documents should be noted. This document was drafted in accordance with the editorial rules of the ISO/IEC Directives, Part 2 (see www.iso.org/directives).

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For an explanation on the meaning of ISO specific terms and expressions related to conformity assessment, as well as information about ISO's adherence to the WTO principles in the Technical Barriers to Trade (TBT) see the following URL: Foreword - Supplementary information.

The committee responsible for this document is ISO/TC 24, *Particle characterization including sieving*, Subcommittee SC 4, *Particle characterization*.

This second edition cancels and replaces the first edition (ISO 9276-2:2001), which has been technically revised.

ISO 9276 consists of the following parts, under the general title *Representation of results of particle size analysis*:

— *Part 1: Graphical representation*

— *Part 2: Calculation of average particle sizes/diameters and moments from particle size distributions*

— *Part 3: Adjustment of an experimental curve to a reference model*

— *Part 4: Characterization of a classification process*

— *Part 5: Methods of calculation relating to particle size analyses using logarithmic normal probability distribution*

— *Part 6: Descriptive and quantitative representation of particle shape and morphology*

Introduction

Particle size analysis is often used for characterization of particulate matter. The relationship between the physical properties of particulate matter, such as powder strength, flowability, dissolution rate, emulsion/suspension stability and particle size forms always the reason for such characterization. For materials having a particle size distribution, it is important to use the relevant parameter, a certain mean particle size, weighted for example by number, area or volume, in the relationship with physical properties.

This part of ISO 9276 describes two procedures for the use of moments for the calculation of mean sizes, the spread and other statistical measures of a particle size distribution.

The first method is named moment-notation. The specific utility of the moment-notation is to characterize size distributions by moments and mean sizes. The moment-notation addresses weighting principles from physics, especially mechanical engineering, and includes arithmetic means from number based distributions only as one part[1][2].

The second method is named moment-ratio-notation. The moment-ratio-notation is based on a number statistics and frequencies approach, but includes also conversion to other types of quantities[3][4].

Important is that the meaning of the subscripts of mean sizes defined in the moment-notation differs from the subscripts of mean sizes defined in the moment-ratio-notation. Both notations are linked by a simple relationship, given in Clause 6.

Both notations are suited for derivation and/or selection of mean sizes related to physical product and process properties for so-called property functions and process functions. The type of mean size to be preferred should have a causal relationship with the relevant physical product or process property.

The particle characterization community embraces a very broad spectrum of science disciplines. The notation of the size distribution employed has been influenced by the branch of industry and the application and thus no single notation has found universal favour.

There are some particle size dependent properties, like light scattering in certain particle size ranges, which cannot be characterized by mean particles sizes, derived from simple power law equations of the notation systems[5].

Representation of results of particle size analysis —

Part 2:
Calculation of average particle sizes/diameters and moments from particle size distributions

1 Scope

This part of ISO 9276 provides relevant equations and coherent nomenclatures for the calculation of moments, mean particle sizes and standard deviations from a given particle size distribution. Two notation systems in common use are described. One is the method of moments while the second describes the moment-ratio method. The size distribution may be available as a histogram or as an analytical function.

The equivalent diameter of a particle of any shape is taken as the size of that particle. Particle shape factors are not taken into account. It is essential that the measurement technique is stated in the report in view of the dependency of sizing results of measurement principle. Samples of particles measured are intended to be representative of the population of particles.

For both notation systems, numerical examples of the calculation of mean particle sizes and standard deviation from histogram data are presented in an annex.

The accuracy of the mean particle size may be reduced if an incomplete distribution is evaluated. The accuracy may also be reduced when very limited numbers of size classes are employed.

2 Normative references

The following documents, in whole or in part, are normatively referenced in this document and are indispensable for its application. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

ISO 9276-1:1998, *Representation of results of particle size analysis — Part 1: Graphical representation*

ISO 9276-5:2005, *Representation of results of particle size analysis — Part 5: Methods of calculation relating to particle size analyses using logarithmic normal probability distribution*

3 Definitions, symbols and abbreviated terms

If necessary, different symbols are given to the moment-notation (M) and the moment-ratio-notation (M-R). This serves the purpose of a clear differentiation between the two systems. For both notation systems, a terminology of specific mean particle sizes is inserted in the corresponding clauses: Clause 4 and Clause 5, respectively.

M-notation	M-R-notation	Description
i	i	number of the size class with upper particle size: x_i(M) or midpoint particle size D_i(M-R)
k		power of x
m	m	number of size classes

M-notation	M-R-notation	Description
r	r	type of quantity of a distribution (general description)
		$r = 0$, type of quantity: number
		$r = 1$, type of quantity: length
		$r = 2$, type of quantity: surface or projected area
		$r = 3$, type of quantity: volume or mass
$M_{k,r}$		complete k-th moment of a $q_r(x)$ – sample distribution
$m_{k,r}$		complete k-th central moment of a $q_r(x)$ – sample distribution
	M_p	p-th moment of a number distribution density
	m_p	p-th central moment of a number distribution density
	N	total number of particles in a sample
	O	order of a mean particle size ($O = p + q$)
	p, q	powers of D in moments or subscripts indicating the same
$q_r(x)$	$q_r(D)$	distribution density of type of particle quantity r
$\bar{q}_{r,i}$		mean height of a distribution density in the i-th particle size interval, Δx_i
$Q_r(x)$	$Q_r(D)$	cumulative distribution of type of quantity r
$\Delta Q_{\mathrm{r},i}$		difference of two values of the cumulative distribution, i.e. relative amount in the i-th particle size interval, Δx_i
s_r	s_r	standard deviation of a $q_r(x)$ and $q_r(D)$ distribution
s_g	s_g	geometric standard deviation of a distribution
s	s	standard deviation of lognormal distribution ($s = \ln s_g$)
S	S	surface area
S_V	S_V	volume specific surface area
V	V	particle volume
$\bar{V}$		mean particle volume
x	D	particle size, diameter of an equivalent sphere
x_i		upper particle size of the i-th particle size interval
$x_{i\text{-}1}$		lower particle size of the i-th particle size interval
	D_i	midpoint size of the i-th size class
$x_{\min}$		particle size below which there are no particles in a given size distribution

M-notation	M-R-notation	Description
x_{max}		particle size above which there are no particles in a given size distribution
$\bar{x}_{k,r}$	$\bar{D}_{p,q}$	mean particle sizes (general description)
	$\bar{D}_{p,p}$	geometric mean particle sizes
$\bar{x}_{k,0}$		arithmetic mean particle size
$\bar{x}_{k,r}$		weighted mean particle size
$\bar{x}_{geo,r}$		geometric mean particle size
$\bar{x}_{har,r}$		harmonic mean particle size
$x_{50,3}$		median particle size of a cumulative volume distribution
$\Delta x_i = x_i - x_{i\text{-}1}$		width of the *i*-th particle size interval

4 The moment-notation

Moments are the basis for defining mean sizes and standard deviations of particle size distributions. A random sample, containing a limited number of particles from a large *population* of particle sizes, is used for estimation of the moments of the size distribution of that population. Estimation is concerned with inference about the numerical values of the unknown population from those of the sample. Particle size measurements are always done on discrete samples and involve a number of discrete size classes. Therefore, only moments related to samples are dealt with in this part of ISO 9276.

4.1 Definition of moments according to the moment-notation

The complete *k*-th moment of a distribution density[1] is represented by integrals as defined in Formula (1). *M* stands for moment. The first subscript, *k*, of *M* indicates the power of the particle size *x*, the second subscript, *r*, of *M* describes the type of quantity of the distribution density.

$$M_{k,r} = \int_{x_{min}}^{x_{max}} x^k q_r(x) \mathrm{d}x \qquad (1)$$

If $r = 0$, $q_0(x)$ represents a number distribution density, if $r = 3$, $q_3(x)$ represents a volume or mass distribution density.

Formula (1) describes a *complete moment* if the integral boundaries are represented by the minimum particle size (x_{min}) and the maximum particle size (x_{max}).

A special complete moment is represented by $M_{0,r}$:

$$M_{0,r} = \int_{x_{\min}}^{x_{\max}} x^0 q_r(x)\mathrm{d}x = \int_{x_{\min}}^{x_{\max}} q_r(x)\mathrm{d}x = Q_r(x_{\max}) - Q_r(x_{\min}) = 1 \qquad (2)$$

with

$$Q_r(x_i) = \int_{x_{\min}}^{x_i} q_r(x)dx \qquad (3)$$

A moment is *incomplete*, if the integration is performed between two arbitrary particle diameters $x_{i\text{-}1}$ and x_i within the given size range of a distribution:

$x_{\min} < x_{i\text{-}1} < x < x_i < x_{\max}$

$$M_{k,r}(x_{i-1}, x_i) = \int_{x_{i-1}}^{x_i} x^k q_r(x)\mathrm{d}x \qquad (4)$$

Apart from the moments related to the origin of the particle size axis and shown in Formulae (1) and (4), the so-called k-th *central moment of* a $q_r(x)$ – distribution density, $m_{k,r}$, can be derived from a given distribution density. It is related to the weighted mean particle size $\bar{x}_{k,r}$ [see Formula (11)].

The *complete* k-th *central moment* is defined as:

$$m_{k,r} = \int_{x_{\min}}^{x_{\max}} (x - \bar{x}_{1,r})^k q_r(x)\mathrm{d}x \qquad (5)$$

4.2 Definition of mean particle sizes according to the moment-notation

All *mean particle sizes* are defined by Formula (6):

$$\bar{x}_{k,r} = \sqrt[k]{M_{k,r}} \qquad (6)$$

Depending on the numbers chosen for the subscripts, k and r, different mean particle sizes may be defined. Since the mean particle sizes calculated from Formula (6) may differ considerably, the subscripts k and r should always be quoted.

There are two groups of mean particle sizes, which should preferably be used, viz. arithmetic mean particle sizes and weighted mean particle sizes.

4.2.1 Terminology for mean particle sizes in the moment-notation $\bar{x}_{k,r}$

Table 1 presents terminology examples of mean sizes.

Table 1 — Terminology for mean particle sizes $\bar{x}_{k,r}$

Systematic code	Terminology
$\bar{x}_{1,0}$	arithmetic mean size
$\bar{x}_{2,0}$	arithmetic mean area size
$\bar{x}_{3,0}$	arithmetic mean volume size
$\bar{x}_{1,1}$	size-weighted mean size
$\bar{x}_{1,2}$	area-weighted mean size, Sauter mean diameter
$\bar{x}_{1,3}$	volume-weighted mean size

4.2.2 Arithmetic mean particle sizes

Arithmetic mean size is a number-weighted mean size, calculated from a number distribution density, $q_0(x)$:

$$\bar{x}_{k,0} = \sqrt[k]{M_{k,0}} \tag{7}$$

Counting single particles in a microscope image is a typical example to obtain number ($r = 0$) percentages as basis of averaging.

In accordance with Reference [2], the recommended mean particle sizes are:

arithmetic mean size (corresponds to arithmetic mean length size):

$$\bar{x}_{1,0} = M_{1,0} \tag{8}$$

arithmetic mean area size (Heywood[2]: mean surface diameter):

$$\bar{x}_{2,0} = \sqrt[2]{M_{2,0}} \tag{9}$$

arithmetic mean volume size (Heywood[2]: mean-weight diameter):

$$\bar{x}_{3,0} = \sqrt[3]{M_{3,0}} \tag{10}$$

4.2.3 Weighted mean particle sizes

Weighted mean particle sizes are defined by:

$$\bar{x}_{k,r} = \sqrt[k]{M_{k,r}} \tag{11}$$

Weighing sieves before and after sieving is a typical example to obtain mass ($r = 3$) percentages as basis of averaging. Weighted mean particle sizes represent the abscissa of the centre of gravity of a $q_r(x)$ – distribution. The recommended weighted mean particle sizes are represented by Formulae (12) to (15).

The weighted mean particle size of a number distribution density, $q_0(x)$, is equivalent to the arithmetic mean length size [see Formula (8)]. It is represented by:

arithmetic mean size (Heywood[6]: numerical mean diameter):

$$\bar{x}_{1,0} = M_{1,0} \tag{12}$$

The weighted mean particle size of a length distribution density, $q_1(x)$, is given by:

size-weighted mean size (Heywood[6]: linear mean diameter):

$$\bar{x}_{1,1} = M_{1,1} \tag{13}$$

The weighted mean particle size of a surface distribution density, $q_2(x)$, is represented by:

area-weighted mean size (Heywood[6]: surface mean diameter):

$$\bar{x}_{1,2} = M_{1,2} \tag{14}$$

The weighted mean particle size of a volume distribution density, $q_3(x)$, is given by:

volume-weighted mean size (Heywood[6]: weight mean diameter):

$$\bar{x}_{1,3} = M_{1,3} \tag{15}$$

4.2.4 Geometric mean particle sizes

If a particle size distribution conforms satisfactorily to a lognormal size distribution (see ISO 9276-5), the geometric mean particle size characterizes the mean value of the logarithm of x. The median of a lognormal distribution has the same value as the geometric mean size.

Instead of the arithmetic mean, calculated from the sum of n values, divided by their number n, the geometric mean is the n-th root of the product of n values. In terms of logarithms the logarithm of the geometric mean is calculated from the sum of the logarithms of n values, divided by their number n. The arithmetic mean is greater than the geometric, the inequality increasing the greater the dispersion among the values.

Mathematical limit analysis of Formula (6) with k approaching zero (see also derivation for $p = q$ in moment-ratio-notation[3]) leads to the geometric mean size:

$$\bar{x}_{0,r} = e^{\int_{x_{\min}}^{x_{\max}} \ln x \, q_r(x) dx} = \bar{x}_{\mathrm{geo},r} \tag{16}$$

or in terms of logarithms:

$$\ln \bar{x}_{0,r} = \ln \bar{x}_{\mathrm{geo},r} = \int_{x_{\min}}^{x_{\max}} \ln x \, q_r(x) dx \tag{17}$$

Based on data from a histogram one obtains the r-weighted geometric mean size:

$$\bar{x}_{0,r} = \exp\left(\sum_{i=1}^{m} \ln \bar{x}_i \, \bar{q}_{r,i} \Delta x_i \right) = \exp\left(\sum_{i=1}^{m} \ln \bar{x}_i \, \Delta Q_{r,i} \right) = \bar{x}_{\mathrm{geo},r} \tag{18}$$

4.2.5 Harmonic mean particle sizes

The harmonic mean of a series of values is the reciprocal of the arithmetic mean of their reciprocals[7]. The harmonic mean is smaller than the geometric, the inequality increasing the greater the dispersion among the values. Therefore the r-weighted harmonic mean size can be calculated from:

$$\bar{x}_{har,r} = \frac{1}{\int_{x_{max}}^{x_{min}} \frac{1}{x} q_r(x) dx} = \frac{1}{M_{-1,r}} \tag{19}$$

or based on data from a histogram:

$$\bar{x}_{har,r} = \frac{1}{\sum_{i=1}^{m} \frac{1}{\bar{x}_i} \bar{q}_{r,i} \Delta x_i} = \frac{1}{\sum_{i=1}^{m} \frac{1}{\bar{x}_i} \Delta Q_{r,i}} \tag{20}$$

4.3 Calculation of moments and mean particle sizes from a given size distribution

4.3.1 The calculation of $M_{k,r}$ and mean particle sizes from a number or a volume based size distribution

In many cases of practical application, the measured data are either represented by a number distribution density, $q_0(x)$, or a volume distribution density, $q_3(x)$. The calculation of the mean particle sizes described above can then be performed according to Formula (21)[1]:

$$\bar{x}_{k,r} = \sqrt[k]{M_{k,r}} = \sqrt[k]{\frac{M_{k+r,0}}{M_{r,0}}} = \sqrt[k]{\frac{M_{k+r-3,3}}{M_{r-3,3}}} \tag{21}$$

This leads to:

$$\bar{x}_{2,0} = \sqrt{M_{2,0}} = \sqrt{\frac{M_{-1,3}}{M_{-3,3}}} \tag{22}$$

$$\bar{x}_{3,0} = \sqrt[3]{M_{3,0}} = \sqrt[3]{\frac{1}{M_{-3,3}}} \tag{23}$$

$$\bar{x}_{1,1} = M_{1,1} = \frac{M_{2,0}}{M_{1,0}} = \frac{M_{-1,3}}{M_{-2,3}} \tag{24}$$

$$\bar{x}_{1,2} = M_{1,2} = \frac{M_{3,0}}{M_{2,0}} = \frac{1}{M_{-1,3}} \tag{25}$$

$$\bar{x}_{1,3} = M_{1,3} = \frac{M_{4,0}}{M_{3,0}} \tag{26}$$

One realizes from Formulae (21) to (26), that the following moments are needed if the mean particle sizes defined above are to be calculated:

from a given number distribution density, $q_0(x)$: $M_{1,0}$; $M_{2,0}$; $M_{3,0}$; $M_{4,0}$

from a given volume distribution density, $q_3(x)$: $M_{1,3}$ $M_{-1,3}$; $M_{-2,3}$; $M_{-3,3}$

Formula (21) shows, that each mean particle size or moment of a given type of quantity can be expressed as a ratio of two number based moments, which is used as the main approach of the moment-ratio-notation.

4.3.2 Calculation of $M_{k,r}$ from a particle size distribution, given as a histogram

If a distribution density is given as a histogram, $q_r(x_{i-1}, x_i)$ is constant in the particle size interval $\Delta x_i = x_i - x_{i-1}$.

Formula (1) may therefore be rewritten as follows:

$$M_{k,r} = \int_{x_{\min}}^{x_{\max}} x^k q_r(x) dx = \sum_{i=1}^{m} \bar{x}_i^k \bar{q}_{r,i} \Delta x_i \tag{27}$$

One obtains with

$$\bar{q}_{r,i} = \frac{\Delta Q_{r,i}}{x_i - x_{i-1}} \tag{28}$$

$$M_{k,r} = \int_{x_{\min}}^{x_{\max}} x^k q_r(x) dx = \sum_{i=1}^{m} \bar{x}_i^k \Delta Q_{r,i} \tag{29}$$

The approximate mean $\bar{x}_i^k$ within a size class can be calculated as arithmetic mean in each size class

$$\bar{x}_i^k = \left(\frac{x_i + x_{i-1}}{2} \right)^k \tag{30}$$

Alternative approximate means like geometric mean or an integral mean have not specific advantage. Several investigations have shown (see e.g. Reference [8]), that there is no general preference for all types of distributions possible.

The discrete nature of histogram data causes uncertainties up to a few percent in the calculated moments and mean sizes, which relate to the width of the size classes and the corresponding uncertainty in the amount of particles derived from the estimated mean size in each class. Methods to improve the size resolution of the representation of measurement by observation of more size classes are given in ISO 9276-3.

The moments $M_{1,0}$, $M_{2,0}$, $M_{3,0}$, $M_{4,0}$, $M_{1,3}$, $M_{-1,3}$, $M_{-2,3}$ and $M_{-3,3}$ can therefore be calculated from Formulae (31) to (38):

$$M_{1,0} = \sum_{i=1}^{m} \bar{x}_i^1 \bar{q}_{0,i} \Delta x_i = \sum_{i=1}^{m} \bar{x}_i^1 \Delta Q_{0,i} \tag{31}$$

$$M_{2,0} = \sum_{i=1}^{m} \bar{x}_i^2 \bar{q}_{0,i} \Delta x_i = \sum_{i=1}^{m} \bar{x}_i^2 \Delta Q_{0,i} \tag{32}$$

$$M_{3,0} = \sum_{i=1}^{m} \bar{x}_i^3 \bar{q}_{0,i} \Delta x_i = \sum_{i=1}^{m} \bar{x}_i^3 \Delta Q_{0,i} \tag{33}$$

$$M_{4,0} = \sum_{i=1}^{m} \bar{x}_i^4 \bar{q}_{0,i} \Delta x_i = \sum_{i=1}^{m} \bar{x}_i^4 \Delta Q_{0,i} \tag{34}$$

$$M_{1,3} = \sum_{i=1}^{m} \bar{x}_i^1 \bar{q}_{3,i} \Delta x_i = \sum_{i=1}^{m} \bar{x}_i^1 \Delta Q_{3,i} \tag{35}$$

$$M_{-1,3} = \sum_{i=1}^{m} \frac{1}{\bar{x}_i^1} \bar{q}_{3,i} \Delta x_i = \sum_{i=1}^{m} \frac{1}{\bar{x}_i^1} \Delta Q_{3,i} \tag{36}$$

$$M_{-2,3} = \sum_{i=1}^{m} \frac{1}{\bar{x}_i^2}\, \bar{q}_{3,i}\, \Delta x_i = \sum_{i=1}^{m} \frac{1}{\bar{x}_i^2}\, \Delta Q_{3,i} \tag{37}$$

$$M_{-3,3} = \sum_{i=1}^{m} \frac{1}{\bar{x}_i^3}\, \bar{q}_{3,i}\, \Delta x_i = \sum_{i=1}^{m} \frac{1}{\bar{x}_i^3}\, \Delta Q_{3,i} \tag{38}$$

4.4 Variance and standard deviation of a particle size distribution

The spread of a size distribution may be represented by its variance, which represents the square of the standard deviation, s_r.. The variance, s_r^2, of a $q_r(x)$ – distribution is defined as:

$$s_r^2 = \int_{x_{\min}}^{x_{\max}} \left(x - \bar{x}_{1,r}\right)^2 q_r(x)\, dx \tag{39}$$

Introducing complete moments, the variance can be calculated (Reference [3]) from:

$$s_r^2 = m_{2,r} = M_{2,r} - \left(M_{1,r}\right)^2 \tag{40}$$

or based on data from a histogram:

$$s_r^2 = \sum_{i=1}^{m} \bar{x}_i^2\, \bar{q}_{r,i}\, \Delta x_i - \left(\sum_{i=1}^{m} \bar{x}_i^1\, \bar{q}_{r,i}\, \Delta x_i\right)^2 = \sum_{i=1}^{m} \bar{x}_i^2\, \Delta Q_{r,i} - \left(\sum_{i=1}^{m} \bar{x}_i^1\, \Delta Q_{r,i}\right)^2 \tag{41}$$

A numerical example of the calculation of s_r^2 is given in Annex A.

For a lognormal $q_r(x)$ – distribution, the standard deviation s can be calculated from:

$$s = \ln(x_{84,r} / x_{50,r}) = \ln(x_{50,r} / x_{16,r}) \tag{42}$$

The geometrical standard deviation s_g is obtained from:

$$s_g = \exp(s) \tag{43}$$

Hence,

$$s_g = x_{84,r} / x_{50,r} = x_{50,r} / x_{16,r} \tag{44}$$

4.5 Calculation of moments and mean particle sizes from a lognormal distribution

The *complete* k-th moment of a lognormal probability distribution, $q_r(x)$, calculates to

$$M_{k,r} = x_{50,r}{}^{k}\, e^{0{,}5\, k^2 s^2} = e^{k \ln x_{50,r} + 0{,}5\, k^2 s^2} \tag{45}$$

A series of mean particle sizes can be calculated from the k-th root of the k-th moment in Formula (45) or from the median (and geometric mean) $x_{50,r}$ and the standard deviation of that distribution using Formula (46):

$$\bar{x}_{k,r} = x_{50,r}\, e^{0{,}5\, k\, s^2} = e^{\ln x_{50,r} + 0{,}5\, k\, s^2} \tag{46}$$

The median $x_{50,r}$ of a lognormal distribution has the same value as the geometric mean size $\bar{x}_{0,r}$.

4.6 Calculation of volume specific surface area and the Sauter mean diameter

From distributions of any type of quantity moments can be used in the calculation of the *volume specific surface area*, S_V, since S_V is inversely proportional to the weighted mean surface size, the Sauter mean diameter, $\bar{x}_{1,2}$ (Formula 14). It is given by:

$$S_V = \frac{6}{\bar{x}_{1,2}} \tag{47}$$

Taking into account Formula (25), one arrives from surface, number or volume distributions at:

$$S_V = \frac{6}{M_{1,2}} = 6\frac{M_{2,0}}{M_{3,0}} = 6 \cdot M_{-1,3} \tag{48}$$

For particles other than spheres a shape factor shall be introduced.

5 The moment-ratio-notation

Moments are the basis for defining mean sizes and standard deviations of particle size distributions. A *random sample*, containing a limited number of particles from a large *population* of particle sizes, is used for estimation of the moments of the size distribution of that population. Estimation is concerned with inference about the numerical values of the unknown population from those of the sample. Particle size measurements are always done on discrete samples and involve a number of discrete size classes. Therefore, only moments related to samples are dealt with in this part of ISO 9276.

NOTE Distribution density and cumulative distribution are represented by q and Q in the ISO 9276 series, but in literature (References [3],[4],[7]–[9]) the symbols f and F are also used.

5.1 Definition of moments according to the moment-ratio-notation

Two different types of moments may be used, viz., *moments* and *central moments*. Moments are centred around the origin of the particle size axis and central moments around the arithmetic mean particle size.

The p-th *moment* of a sample, denoted as M_p, is defined as:

$$M_p = N^{-1} \sum_i n_i \, D_i^p \tag{49}$$

where

$N = \sum_i n_i$ is the total number of particles involved in the measurement;

D_i is the midpoint of the i-th size class [see also comments to Formula (30)];

n_i is the number of particles in the i-th size class (i.e. the class frequency of the number distribution density).

The first *moment*, the (arithmetic) sample mean M_1 of the particle sizes D, is mostly represented by $\bar{D}$. The second and third *moments* are proportional to the mean surface area and the mean volume respectively, of the particles in a sample.

The p-th *central moment* around the mean $\bar{D}$, denoted as m_p, is defined by:

$$m_p = N^{-1} \sum_i n_i (D_i - \bar{D})^p \tag{50}$$

Central moments of particle sizes D, are related to differences from the mean value. The best-known example is the sample variance m_2.

5.2 Definition of mean particle sizes according to the moment-ratio-notation

The mean particle size $\bar{D}_{p,q}$ of a sample of particle sizes is the $1/(p - q)$-th power of the ratio of the p-th and the q-th moment of the number distribution density of the sample of particle sizes (see Reference [5]):

$$\bar{D}_{p,q} = \left[\frac{M_p}{M_q} \right]^{1/(p-q)} \quad , \text{if } p \neq q \tag{51}$$

Using Formula (49), Formula (51) can be rewritten as:

$$\bar{D}_{p,q} = \left[\frac{\sum_i n_i D_i^p}{\sum_i n_i D_i^q} \right]^{1/(p-q)} \quad , \text{if } p \neq q \tag{52}$$

For equal values of p and q, Formula (53) holds (see Reference [5]):

$$\bar{D}_{p,p} = \exp \left[\frac{\sum_i n_i D_i^p \ln D_i}{\sum_i n_i D_i^p} \right] \tag{53}$$

The powers p and q may have any numerical value. The type of mean size to be preferred should have a causal relationship with the relevant physical product or process property[4],[10].

5.2.1 Terminology for mean particle sizes in the moment-ratio-notation $\bar{D}_{p,q}$

Table 2 presents the M-R terminology of mean sizes[9].

Table 2 — Terminology for mean particle sizes $\bar{D}_{p,q}$

Systematic code	Terminology
$\bar{D}_{-3,0}$	arithmetic harmonic mean volume size
$\bar{D}_{-2,1}$	size-weighted harmonic mean volume size
$\bar{D}_{-1,2}$	area-weighted harmonic mean volume size
$\bar{D}_{-2,0}$	arithmetic harmonic mean area size
$\bar{D}_{-1,1}$	size-weighted harmonic mean area size
$\bar{D}_{-1,0}$	arithmetic harmonic mean size

Table 2 *(continued)*

Systematic code	Terminology
$\bar{D}_{0,0}$	arithmetic geometric mean size
$\bar{D}_{1,1}$	size-weighted geometric mean size
$\bar{D}_{2,2}$	area-weighted geometric mean size
$\bar{D}_{3,3}$	volume-weighted geometric mean size
$\bar{D}_{1,0}$	arithmetic mean size
$\bar{D}_{2,1}$	size-weighted mean size
$\bar{D}_{3,2}$	area-weighted mean size, Sauter mean diameter
$\bar{D}_{4,3}$	volume-weighted mean size
$\bar{D}_{2,0}$	arithmetic mean area size
$\bar{D}_{3,1}$	size-weighted mean area size
$\bar{D}_{4,2}$	area-weighted mean area size
$\bar{D}_{5,3}$	volume-weighted mean area size
$\bar{D}_{3,0}$	arithmetic mean volume size
$\bar{D}_{4,1}$	size-weighted mean volume size
$\bar{D}_{5,2}$	area-weighted mean volume size
$\bar{D}_{6,3}$	volume-weighted mean volume size

5.2.2 Geometric mean particle sizes

Table 2 shows that the set of mean sizes $\bar{D}_{p,p}$ are geometric mean particle sizes[9]. An example is the geometric mean surface diameter, $\bar{D}_{2,2}$, for visual ranking of photographs of air bubble size distributions[4].

5.2.3 Harmonic mean particle sizes

Table 2 shows that the set of mean sizes $\bar{D}_{p,q}$ having negative p values are harmonic mean particle sizes[9]. A theoretical example, viz. heat transfer to or from particles, is given in Reference [4].

5.3 Calculation of mean particle sizes from a given size distribution

Mean sizes $\overline{D}_{p,q}$ of a sample can be estimated from any size distribution $q_r(D)$ according to equations similar to Formulae (52) and (53):

$$\overline{D}_{p,q} = \left[\frac{\sum_{i}^{m} q_r(D_i)\, D_i^{p-r}}{\sum_{i}^{m} q_r(D_i)\, D_i^{q-r}} \right]^{\frac{1}{p-q}} \text{, if } p \neq q \tag{54}$$

and

$$\overline{D}_{p,p} = \exp\left[\frac{\sum_{i}^{m} q_r(D_i)\, D_i^{p-r} \ln D_i}{\sum_{i}^{m} q_r(D_i)\, D_i^{p-r}} \right] \text{, if } p = q \tag{55}$$

where

$q_r(D_i)$ is the particle quantity in the i-th class;

D_i is the midpoint of the i-th class interval;

r is equal to 0, 1, 2 or 3 and represents the type of quantity, viz. number, diameter, surface, volume (or mass) respectively;

m is the number of classes.

It is not necessary that the particle quantity $q_r(D_i)$ be a normalized quantity. The quantity can be normalized, however, through: $\Sigma\, q_r(D_i) = 1$. Formulae (54) and (55) reduce to the familiar form of Formulae (52) and (53) when $r = 0$ and $n_i = q_0(D_i)$, i.e. for a number distribution density.

The discrete nature of histogram data causes uncertainties up to a few percent in the calculated moments and mean diameters, which relate to the width of the size classes and the corresponding uncertainty in the amount of particles derived from the estimated mean size in each class. More information is given in Clause 7.

5.4 Variance and standard deviation of a particle size distribution

The *central moment* m_2, called variance of a number distribution density (r = 0), is defined by:

$$m_2 = N^{-1} \sum_i n_i \left(D_i - \bar{D}_{1,0}\right)^2 \tag{56}$$

Since m_2 always underestimates the variance σ^2 (squared standard deviation) of the particle sizes in the population, m_2 is multiplied by $N/(N\text{-}1)$ to obtain an unbiased estimator, s^2, for the population variance. Thus, the variance $s_0{}^2$ of the particle sizes in the sample has to be calculated from Formula (57):

$$s_0^2 = \frac{N}{N-1} m_2 = \frac{\sum_i n_i \left(D_i - \bar{D}_{1,0}\right)^2}{N-1} \tag{57}$$

and the standard deviation s_0 from Formula (58):

$$s_0 = \sqrt{\frac{\sum_i n_i D_i^2 - N \bar{D}_{1,0}^2}{N-1}} \tag{58}$$

Formula (58) may be rewritten as:

$$s_0 = c \sqrt{\bar{D}_{2,0}^2 - \bar{D}_{1,0}^2} \tag{59}$$

with

$$c = \sqrt{N/(N-1)} \tag{60}$$

In practice, if $N >> 100$, then $c \approx 1$ and hence

$$s_0 \approx \sqrt{\bar{D}_{2,0}^2 - \bar{D}_{1,0}^2} \tag{61}$$

Formula (61) holds for number distribution density (r = 0). Generally, for any distribution density $q_r(D)$ the standard deviation, s_r, can be calculated from Formula (62), although s_r is not unbiased[3]:

$$s_r \approx \sqrt{\bar{D}_{2+r,r}^2 - \bar{D}_{1+r,r}^2} \tag{62}$$

A numerical example of the calculation of s_r^2 is given in Annex B.

The *population* standard deviation σ of a lognormal distribution of particle sizes can be estimated by the *sample* standard deviation s:

$$s = \sqrt{\frac{\sum_i n_i \left\{ \ln\left(D_i / \bar{D}_{0,0}\right) \right\}^2}{N-1}} \tag{63}$$

Note that in this case σ and s are standard deviations of log-transformed particle sizes D.

Analogous to Formula (62), for any lognormal distribution density $q_r(D)$ the standard deviation, s, can be calculated from Formula (64), although s is not unbiased:

$$s = \sqrt{\frac{\sum_i n_i D_i^r \left\{ \ln(D_i / \overline{D}_{r,r}) \right\}^2}{\sum_i n_i D_i^r}} \tag{64}$$

In particle size analysis, the quantity s_g,

$$s_g = \exp[s] \tag{65}$$

is referred to as the geometric standard deviation[3] although it is not a standard deviation in its true sense.

5.5 Relationships between mean particle sizes

It can be shown (see Reference [5]) that

$$\overline{D}_{p,0} \le \overline{D}_{m,0} \text{ , if } p \le m \tag{66}$$

and

$$\overline{D}_{p-1,q-1} \le \overline{D}_{p,q} \tag{67}$$

Differences between mean sizes decrease as the uniformity of the particle sizes D increases. The equal sign is applicable when all particles are of the same size.

An alternative relationship for relating several mean particle sizes has the form

$$\left[\overline{D}_{p,q}\right]^{p-q} = \overline{D}_{p,0}^{p} / \overline{D}_{q,0}^{q} \tag{68}$$

For example when $p = 3$ and $q = 2$: $\overline{D}_{3,2} = \overline{D}_{3,0}^{3} / \overline{D}_{2,0}^{2}$.

Formula (69) represents a simple symmetry relationship:

$$\overline{D}_{p,q} \equiv \overline{D}_{q,p} \tag{69}$$

The sum O of the subscripts p and q is called the order of the mean size $\overline{D}_{p,q}$:

$$O = p + q \tag{70}$$

For lognormal particle-size distributions, the following relationship between mean sizes is applicable:

$$\overline{D}_{p,q} = \overline{D}_{0,0} \exp[(p+q)s^2/2] \tag{71}$$

The accuracy of Formula (71) is about 2 % if, e.g. the standard deviation s = 0,7, the order O (= $p + q$) of $\overline{D}_{p,q}$ is 6 and the sample size N = 180 particles; or if s = 1,0, O = 10 and N = 1 450 particles. A smaller standard deviation s, lower order O or larger sample size N results in a better accuracy of the calculated $\overline{D}_{p,q}$ value.

Formula (71) shows that for lognormal size distributions, the values of mean sizes of the same order *O* are equal. From Formula (71), follows that:

$$\bar{D}_{p,q} = \bar{D}_{3,3} \exp[(p+q-6)\,s^2/2] \tag{72}$$

5.6 Calculation of volume specific surface area and the Sauter mean diameter

The *volume specific surface area*, S_V, is inversely proportional to the surface-weighted mean diameter, $\bar{D}_{3,2}$, (also called Sauter mean diameter). It is given by:

$$S_V = \frac{6}{\bar{D}_{3,2}} \tag{73}$$

For particles, other than spheres, a shape factor has to be introduced.

6 Relationship between moment-notation and moment-ratio-notation

In some application areas the M-notation is preferred, while in other areas the preference is for the M-R-notation. Both methods differ in symbols and terminology, as shown in Clauses 3, 4, 5, but use similar calculation methods. Between the mean particle sizes $\bar{x}_{k,r}$ and $\bar{D}_{p,q}$ of both notations exists the relationship given by Formula (74):

$$\bar{D}_{p,q} = \bar{D}_{k+r,r} = \bar{x}_{k,r} \quad \text{if } q = r \text{ and } p = k + r \tag{74}$$

The condition $k = 0$ describes the geometric mean particle sizes $\bar{x}_{0,r}$, which can be derived in the same way as for $\bar{D}_{q,q}$ in Reference [5].

An example of Formula (74) is the mean particle size related to the volume specific surface area, the Sauter mean diameter: $\bar{D}_{3,2} = \bar{x}_{1,2}$

$$\bar{D}_{3,2} = \left[\frac{\sum_i n_i D_i^3}{\sum_i n_i D_i^2}\right]^{1/(3-2)} = \bar{x}_{1,2} = M_{1,2} = \frac{M_{3,0}}{M_{2,0}} = \frac{1}{M_{-1,3}} \tag{75}$$

The notation for a number distribution density shows the best coincidence between the two notations with $q = r = 0$ and $p = k + 0$:

$$\bar{D}_{p,q} = \left[\frac{\sum_i n_i D_i^p}{\sum_i n_i D_i^q}\right]^{1/(p-q)} \tag{49}$$

and

$$\bar{x}_{k,r} = \sqrt[k]{M_{k,r}} = \sqrt[k]{\frac{M_{k+r,0}}{M_{r,0}}} \tag{61}$$

$$\bar{D}_{1,0} = \bar{x}_{1,0} = M_{1,0} \tag{8}$$

$$\bar{D}_{2,0} = \bar{x}_{2,0} = \sqrt[2]{M_{2,0}} \tag{9}$$

$$\bar{D}_{3,0} = \bar{x}_{3,0} = \sqrt[3]{M_{3,0}} \qquad (10)$$

$$\bar{D}_{2,1} = \bar{x}_{1,1} = M_{1,1} = \frac{M_{2,0}}{M_{1,0}} = \frac{M_{-1,3}}{M_{-2,3}} \qquad (24)$$

$$\bar{D}_{4,3} = \bar{x}_{1,3} = M_{1,3} = \frac{M_{4,0}}{M_{3,0}} \qquad (26)$$

Table 3 presents the systematic codes from the moment-ratio-notation[9] from 5.2.1 in comparison to the moment-notation from 4.2.1.

Table 3 — Terminology for mean particle sizes and corresponding codes of the notation systems

Systematic code M-R-notation	Terminology	Systematic code M-notation
$\bar{D}_{-3,0}$	arithmetic harmonic mean volume size	$\bar{x}_{-3,0}$
$\bar{D}_{-2,1}$	size-weighted harmonic mean volume size	$\bar{x}_{-3,1}$
$\bar{D}_{-1,2}$	area-weighted harmonic mean volume size	$\bar{x}_{-3,2}$
$\bar{D}_{-2,0}$	arithmetic harmonic mean area size	$\bar{x}_{-2,0}$
$\bar{D}_{-1,1}$	size-weighted harmonic mean area size	$\bar{x}_{-2,1}$
$\bar{D}_{-1,0}$	arithmetic harmonic mean size	$\bar{x}_{\text{har},0}$ $(\bar{x}_{-1,0})$
$\bar{D}_{0,0}$	arithmetic geometric mean size	$\bar{x}_{\text{geo},0}$ $(\bar{x}_{0,0})$
$\bar{D}_{1,1}$	size-weighted geometric mean size	$\bar{x}_{0,1}$
$\bar{D}_{2,2}$	area-weighted geometric mean size	$\bar{x}_{0,2}$
$\bar{D}_{3,3}$	volume-weighted geometric mean size	$\bar{x}_{0,3}$
$\bar{D}_{1,0}$	arithmetic mean size	$\bar{x}_{1,0}$
$\bar{D}_{2,1}$	size-weighted mean size	$\bar{x}_{1,1}$
$\bar{D}_{3,2}$	area-weighted mean size, Sauter mean diameter	$\bar{x}_{1,2}$
$\bar{D}_{4,3}$	volume-weighted mean size	$\bar{x}_{1,3}$
$\bar{D}_{2,0}$	arithmetic mean area size	$\bar{x}_{2,0}$

Table 3 *(continued)*

Systematic code M-R-notation	Terminology	Systematic code M-notation
$\bar{D}_{3,1}$	size-weighted mean area size	$\bar{x}_{2,1}$
$\bar{D}_{4,2}$	area-weighted mean area size	$\bar{x}_{2,2}$
$\bar{D}_{5,3}$	volume-weighted mean area size	$\bar{x}_{2,3}$
$\bar{D}_{3,0}$	arithmetic mean volume size	$\bar{x}_{3,0}$
$\bar{D}_{4,1}$	size-weighted mean volume size	$\bar{x}_{3,1}$
$\bar{D}_{5,2}$	area-weighted mean volume size	$\bar{x}_{3,2}$
$\bar{D}_{6,3}$	volume-weighted mean volume size	$\bar{x}_{3,3}$

7 Accuracy of calculated particle size distribution parameters

Any of the below points can cause particle size distributions and their characteristic values to differ significantly if they come from different techniques.

For instance when comparing results from different techniques, it is necessary to convert particle size distribution parameters, such as mean sizes or distribution percentile values, from one type of measured size distribution into another type, e.g. from a volume-based distribution into a number-based distribution. Mathematically, these conversions typically can be done with an accuracy of within 1 %. However, the errors in the parameters are strongly increased by the following:

— if the size distribution is truncated by small cut-offs at either end of the distribution (e.g. 0,05 – 0,3 % *r*/*r*), often applied in view of limited measurement precision or deconvolution problems);

— if the measured size distribution contains only few particles at the upper size end, which quantities therefore have a great uncertainty;

— if the size distribution contains phantom peaks due to presence of heterogeneities within the particles sample or to application of inaccurate models for conversion of measured signals into a size distribution;

— if the type of size distribution (dimensionality *r*) is changed considerably in the conversion of wide size distributions; *(*volume to surface gives lower errors than volume to number*)*

— if the size distribution contains only few, wide size classes;

— if significant measurement errors are present.

Further explanations and examples are given in Annex C.

Annex A
(informative)

Numerical example for calculation of mean particle sizes and standard deviation from a histogram of a volume based size distribution

The cumulative volume distribution in the following numerical example follows a *lognormal distribution* (see ISO 9276-5):

$$q_3(x) = \frac{1}{x\,s\sqrt{2\pi}} \exp\left[-0{,}5\left(\frac{\ln(x/\bar{x}_{0,3})}{s}\right)^2\right] \tag{A.1}$$

where $\bar{x}_{0,3}$ is the *geometric mean diameter* of the volume distribution and s is its *standard deviation* (i.e. of the logarithmic transformed particle sizes). In this case, the value of $\bar{x}_{0,3}$ is equal to the value of the median $x_{50,3}$. The *geometric standard deviation* s_g is:

$$s_g = \exp(s) \tag{A.2}$$

Table A.1 has been calculated under the assumption that the volume distribution has a geometric mean diameter $\bar{x}_{0,3}$ = 5,0 µm and a standard deviation s = 0,50, corresponding to a geometric standard deviation s_g = 1,648 7. For reasons of convenience the successive particle size class boundaries were assumed to follow the R5 series and the R10 series (in practice the number of classes is mostly larger):

$$\text{R5 series: } \frac{x_i}{x_{i-1}} = \sqrt[5]{10} = 1{,}585 \text{ and R10 series: } \frac{x_i}{x_{i-1}} = \sqrt[10]{10} = 1{,}259 \tag{A.3}$$

The upper boundary of the distribution is assumed to be 25,0 µm. The truncated volume fraction above this boundary is 0,000 64. The distribution is also truncated at the lower boundary of the seventh class of the R5 series, being 0,995 27 µm. The truncated volume fraction below this boundary is 0,000 62. The total truncated volume fraction is thus 0,001 26.

The numbers in Table A.1 for x_i; $Q_{3,i}$; Δx_i; $\Delta_{3,i}$, $\Delta Q_{3,i}$ (normalized) and $\bar{q}_{3,i}$ (R5 series) have been used to calculate the moments represented by Formulae (35) to (38). Note that the Q_3 data are not normalized, due to the truncation of the distribution. The Excel[1)] function LOGNORMDIST(x,mean,standard_dev) was used to calculate the $Q_{3,i}$ - values:

$$Q_{3,i} = \text{LOGNORMDIST}(x_i,\ \ln(\bar{x}_{0,3}),\ s) = \text{LOGNORMDIST}(x_i;\ 1{,}609\ 44;0{,}5) \tag{A.4}$$

The analytical values of the moments have been calculated by introducing the lognormal distribution into Formula (1) and integrating between x_{min} = 0 and x_{max} = ∞, i.e. without truncation. The values obtained are given in Table A.2. Column 2 represents the values of the four moments as calculated from the analytical function. Columns 3 and 5 represent the figures obtained in the numerical calculation

1) Excel is the trade name of a product supplied by Microsoft. This information is given for the convenience of users of this document and does not constitute an endorsement by ISO of the product named. Equivalent products may be used if they can be shown to lead to the same results.

using the R5 and the R10 series, respectively. The normalized $\Delta Q_{3,i}$ -values from Table A.1 have to be used for calculation of the columns 3 and 5 values. The calculated data differ slightly from the ones given in column 1, but the agreement remains within a few percent, as shown by the deviations given in columns 4 and 6.

Table A.3 shows the mean particle sizes as calculated from the moments of Table A.2, taking into account Formulae (22) to (26).

The variance s_3^2 of the volume distribution can be calculated according to Formula (43) by using the data in columns 1 and 5 of Table A.1. The values of the midpoints of the size classes are the arithmetic means of two successive class boundary values in column 1 of Table A.1. The value of s_3^2 is 10,081 and the value of the standard deviation s_3 is 3,175.

Table A.1 — Basic data of the lognormal distribution for the calculation of the moments (R5 series)

x_i (µm)	$Q_{3,i}$	Δx_i (µm)	$\Delta Q_{3,i}$	$\Delta Q_{3,i}$ (normalized)	$\bar{q}_{3,i}$ (µm^{-1})
25,000	0,999 4	9,226	0,010 14	0,010 15	0,001 10
15,774	0,989 2	5,821	0,073 50	0,073 59	0,012 64
9,953	0,915 7	3,673	0,240 00	0,240 29	0,065 42
6,280	0,675 7	2,317	0,354 85	0,355 30	0,153 31
3,962	0,320 9	1,462	0,238 04	0,238 35	0,163 00
2,500	0,082 8	0,923	0,072 31	0,072 40	0,078 48
1,577	0,010 5	0,582	0,009 90	0,009 91	0,017 02
0,995	0,000 6				

Table A.2 — Comparison of the analytical and the numerical calculation of the moments

	analytical result	R5-series	deviation R5 (%)	R10-series	deviation R10 (%)
$M_{1,3}$ (µm)	5,666	5,854	3,3	5,703	0,7
$M_{-1,3}$ (µm^{-1})	0,226 6	0,222 2	−2,0	0,225	−0,6
$M_{-2,3}$ (µm^{-2})	0,065 9	0,063 9	−3,1	0,064 9	−1,7
$M_{-3,3}$ (µm^{-3})	0,024 6	0,023 4	−5,1	0,023 6	−4,3

Table A.3 — Comparison of the analytical and the numerical calculation of the mean particle size

	analytical result	R5-series	deviation R5 (%)	R10-series	deviation R10 (%)
$\bar{x}_{1,0}$ (µm)	2,676	2,731	2,1	2,751	2,8
$\bar{x}_{2,0}$ (µm)	3,033	3,082	1,6	3,090	1,9
$\bar{x}_{3,0}$ (µm)	3,436	3,496	1,7	3,487	1,5
$\bar{x}_{1,1}$ (µm)	3,436	3,477	1,2	3,472	1,0
$\bar{x}_{1,2}$ (µm)	4,412	4,501	2,0	4,441	0,7
$\bar{x}_{1,3}$ (µm)	5,666	5,854	3,3	5,703	0,7

The differences in Table A.3 between the analytical results and the results obtained using the R5 and the R10 series are small. In principle the R10-series is to be preferred over the R5-series due to smaller deviations, see especially $\bar{x}_{1,2}$ and $\bar{x}_{1,3}$. They indicate that narrower size classes (as in the R10 series) are to be preferred over wider size classes (as in the R5 series), although differences are fairly small. More information on accuracy is given in Clause 7.

Annex B
(informative)

Numerical example for calculation of mean particle sizes and standard deviation from a histogram of a volume based size distribution

The cumulative volume distribution in the following numerical example follows a *lognormal distribution* (see ISO 9276-5):

$$q_3(D) = \frac{1}{D\,s\sqrt{2\pi}} \exp\left[-0{,}5\left(\frac{\ln(D/\bar{D}_{3,3})}{s}\right)^2\right] \tag{B.1}$$

where $\bar{D}_{3,3}$ is the *volume-weighted geometric mean diameter* of the volume distribution and s is its *standard deviation* (i.e. of the logarithmic transformed particle sizes). The *geometric standard deviation* s_g is:

$$s_g = \exp(s) \tag{B.2}$$

Table B.1 has been calculated under the assumption that the volume distribution has a geometric mean diameter $\bar{D}_{3,3}$ = 5 µm and a standard deviation s = 0,50, corresponding to a geometric standard deviation s_g = 1,648 7. For reasons of convenience the successive particle size class boundaries were assumed to follow the R5 series and the R10 series (in practice the number of classes is mostly larger):

$$\text{R5 series: } \frac{x_i}{x_{i-1}} = \sqrt[5]{10} = 1{,}585 \text{ and R10 series: } \frac{x_i}{x_{i-1}} = \sqrt[10]{10} = 1{,}259 \tag{B.3}$$

The upper boundary of the distribution is assumed to be 25,0 µm. The truncated volume fraction above this boundary is 0,000 64. The distribution is also truncated at the lower boundary of the seventh class of the R5 series, being 0,995 27 µm. The truncated volume fraction below this boundary is 0,000 62. The total truncated fraction is thus 0,001 26. The Excel function LOGNORMDIST(D,mean,standard_dev) was used for calculating values of the cumulative volume fractions $\sum_i n_i D_i^3$ in column 4 of Table B.1 (R5 series):

$$\sum_i n_i D_i^3 = \text{LOGNORMDIST}(Dup_i, \ln(\bar{D}_{3,3}), s) = \text{LOGNORMDIST}(Dup_i;\ 1{,}609\ 44; 0{,}5) \tag{B.4}$$

where Dup_i is the upper boundary of the i-th size class (see column 3). In Table B.1 a slightly different notation for the class boundaries is used to remove any doubts as to the classification. The data in Table B.1 were used to calculate the values in Table B.2. And from these values, which are not based on normalized distributions, mean particle sizes were calculated using Formulae (52) and (53). As the volume distribution is lognormal, the analytical value of any mean particle size of that distribution can be calculated from the values of $\bar{D}_{3,3}$ and s given above, using Formula (72).

Table B.3 shows the calculated mean particle sizes. The differences between the analytical results and the ones obtained using the R10 and the R5 series are small. In principle the R10-series is to be preferred over the R5-series due to smaller deviations, see especially $\bar{D}_{3,2}$ or $\bar{D}_{4,3}$.

Table B.1 — Lognormal volume distribution (R5 series)

Class number	Mid-point D_i [µm]	Range of sizes [µm]	Cum. fraction $\sum_i n_i D_i^3$	Fraction $n_i\, D_i{}^3$
1	1,286	0,995 – < 1,577	0,010 52	0,009 90
2	2,039	1,577 – < 2,500	0,082 83	0,072 31
3	3,231	2,500 – < 3,962	0,320 87	0,238 04
4	5,121	3,962 – < 6,280	0,675 72	0,354 85
5	8,116	6,280 – < 9,953	0,915 71	0,239 99
6	12,863	9,953 – < 15,774	0,989 21	0,073 50
7	20,387	15,774 – < 25,000	0,999 36	0,010 14

Table B.2 gives the relevant data to calculate some mean sizes of the size distribution using Formulae (52) and (53).

Table B.2 — Data to calculate some mean sizes and the geometric standard deviation

Mid-point D_i [µm]	Fraction $n_i\, D_i{}^3$	n_i (× 100)	$n_i \ln D_i$ (× 100)	$n_i\, D_i$ (× 100)	$n_i\, D_i{}^2$ (× 100)	$n_i\, D_i{}^3 \ln D_i$ (× 100)	$n_i\, D_i{}^4$ (× 100)	$n_i\, (\ln(D_i/\bar{D}_{3,3}))^2$ (× 100)
1,286	0,009 90	0,464 9	0,117 1	0,598 1	0,769 3	0,249 2	1,272 9	1,895 2
2,039	0,072 31	0,853 4	0,607 9	1,739 8	3,546 9	5,150 7	14,741 9	6,165 3
3,231	0,238 04	0,705 7	0,827 6	2,280 1	7,367 2	27,918 5	76,914 8	5,099 7
5,121	0,354 85	0,264 2	0,431 6	1,353 1	6,929 4	57,959 4	181,718 4	0,000 2
8,116	0,239 99	0,044 9	0,094 0	0,364 3	2,956 9	50,250 7	194,781 0	5,038 1
12,863	0,073 50	0,003 5	0,008 8	0,044 4	0,571 4	18,774 8	94,545 9	6,203 5
20,387	0,010 14	0,000 1	0,000 4	0,002 4	0,049 7	3,057 7	20,676 3	1,929 2
Sum:	0,998 73	2,336 7	2,0873	6,382 3	22,190 9	163,361 0	584,651 2	26,331 2

Numerical estimates for mean sizes and standard deviation can be calculated by using the sums in the bottom row of Table B.2:

$\bar{D}_{1,0}$ = 6,382 3/2,336 7 = 2,731 [see columns 5, 3, and Formula (52)]

$\bar{D}_{2,0}$ = (22,190 9/2,336 7)$^{1/2}$ = 3,082 [see columns 6, 3, and Formula (52)]

$\bar{D}_{3,0}$ = (99,873/2,336 7)$^{1/3}$ = 3,496 [see columns 2, 3, and Formula (52)]

$\bar{D}_{2,1}$ = 22,190 9/6,383 2 = 3,477 [see columns 6, 5, and Formula (52)]

$\bar{D}_{3,2}$ = 99,873/22,190 9 = 4,501 [see columns 2, 6, and Formula (52)]

$\bar{D}_{4,3}$ = 584,651 2/99,873 = 5,854 [see columns 8, 2, and Formula (52)]

$\bar{D}_{0,0}$ = exp (2,087 3/2,336 7) = 2,443 [see columns 4, 3, and Formula (53)]

$\bar{D}_{3,3}$ = exp (163,361 0/99,873) = 5,133 [see columns 7, 3, and Formula (53)]

$s_g = \exp(s) = \exp\left(\sqrt{26{,}331\,2/(0{,}998\,73\times 100}\right)$ = exp (0,513 47) = 1,671 1 [see columns 9, 2, and Formulae (64) and (65); the sample is assumed to be large, viz. $N >> 100$].

$s_0 = \sqrt{3{,}082^2 - 2{,}731^2} = 1{,}427$ [see the values of $\bar{D}_{2,0}$ and $\bar{D}_{1,0}$ above and Formula (61); the sample is assumed to be large, viz. $N >> 100$].

The values of $\bar{D}_{5,3}$ and $\bar{D}_{4,3}$, being 6,660 (not calculated above) and 5,854 (calculated above), respectively, are required for calculating the standard deviation s_3 of the volume distribution according to Formula (62). From these values follows $s_3 = 3{,}176$ and the variance $s_3^2 = 10{,}086$.

The geometric mean size $\bar{D}_{0,0}$ can be calculated also from the values of $\bar{D}_{3,3} = 5{,}133$ and the logarithm of the geometrical standard deviation s_g: $\ln(s_g) = s = \ln(1{,}671\ 1) = 0{,}513\ 5$, using Formula (72):

$$\bar{D}_{0,0} = 5{,}133 \times \exp((0+0-6) \times 0{,}513\ 5^2/2) = 2{,}327$$

This value deviates about 5 % from the value 2,443 of $\bar{D}_{0,0}$ calculated above using Formula (53), but its deviation from the analytical value is −1,5 %. A comparison of estimates and corresponding analytical values is given in Table B.3.

Table B.3 — Comparison of estimated and analytical values of mean sizes $\bar{D}_{p,q}$ and geometric standard deviation s_g (R5 and R10 series)

Type of mean size and geometric standard deviation	Analytical value [µm]	Estimated value R5 series [µm]	Deviation of R5 series [%]	Estimated value R10 series [µm]	Deviation of R10 series [%]
$\bar{D}_{1,0}$	2,676	2,731	2,06	2,751	2,77
$\bar{D}_{2,0}$	3,033	3,082	1,62	3,090	1,90
$\bar{D}_{3,0}$	3,436	3,496	1,74	3,487	1,48
$\bar{D}_{2,1}$	3,436	3,477	1,18	3,472	1,03
$\bar{D}_{3,2}$	4,412	4,501	2,00	4,441	0,65
$\bar{D}_{4,3}$	5,666	5,854	3,32	5,703	0,66
$\bar{D}_{0,0}$	2,362	2,443	3,44	2,466	4,44
$\bar{D}_{3,3}$	5,000	5,133	2,66	5,033	0,66
s_g	1,648 7	1,583 7	−3,94	1,579 0	−4,23

The differences in Table B.3 between the analytical results and the results obtained using the R5 and the R10 series are small. In principle the R10-series is to be preferred over the R5-series due to smaller deviations, see especially $\bar{D}_{3,2}$, $\bar{D}_{3,3}$ and $\bar{D}_{4,3}$. They indicate that narrower size classes (as in the R10 series) are to be preferred over wider size classes (as in the R5 series), although differences are fairly small. More information on accuracy is given in Clause 7.

Annex C
(informative)

Accuracy of calculated particle size distribution parameters

The width of the size distribution is important since wider distributions cause a larger shift from one type into another type. For example, for the median size of lognormal distributions, ISO 9276-5 states that:

$$\ln(D_{50,3}) = \ln(D_{50,2}) + s^2 = \ln(D_{50,1}) + 2s^2 = \ln(D_{50,0}) + 3s^2 \quad \text{(C.1)}$$

where

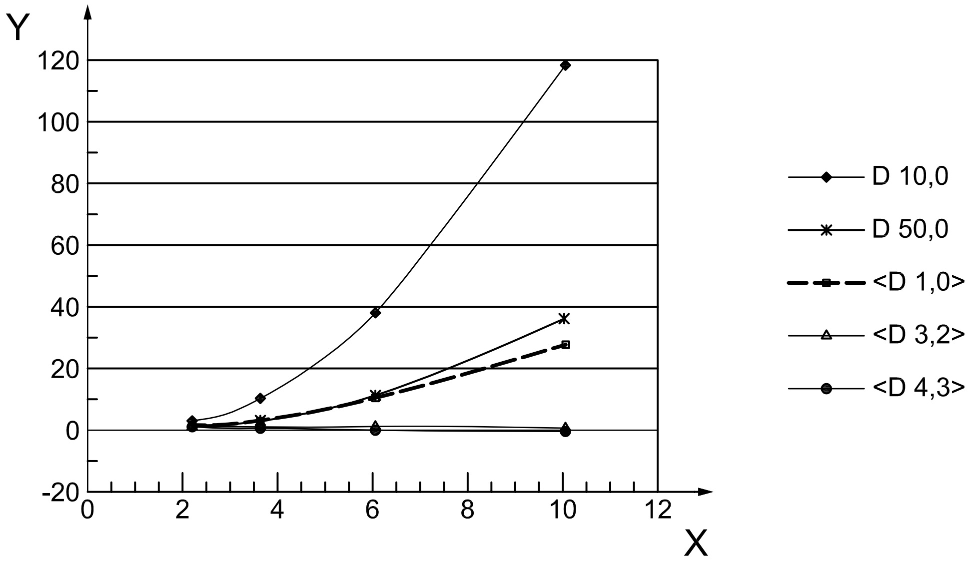
$s = \ln(s_g)$ is the standard deviation of the lognormal distribution;

s_g is the geometric standard deviation of the lognormal distribution.

Similar equations hold for the other characteristic size parameters of the distribution. Formula (C.1) shows that the shift from e.g. $D_{50,3}$ to the $D_{50,0}$ becomes larger if the distributions get wider (i.e. have larger s). For measured (medium-) wide volume-based particle size distributions, it can be calculated that small volume fractions at the lower size end contain a significant number of particles. For example, in a lognormal size distribution having $s = 0{,}7$ (corresponding to $D_{90,3}/D_{10,3} = 6{,}0$), 0,05 % v/v at the small-size end corresponds to 12 % n/n. Thus, a cut-off of 0,05 % v/v here means loss of 12 % of the smallest particles. Similarly, for measured (medium-) wide number-based distributions, a small number of particles at the upper size end relates to a significant volume fraction.

The width of the size classes in a measured particle size distribution becomes important when only a small number of wide size classes is involved in the size distribution, since a wider class means that a larger amount of particles is given the same mean size. Thus, it introduces a larger uncertainty in the conversion from one type of particle size distribution into another type. For example, the R5 data in Annex A and Annex B show a bias up to about 4 %.

As an example, Figure C.1 presents some particle size distribution values, which have been calculated for a volume-based lognormal distribution around $D_{50,3} = 5$ µm at different size distribution widths. The theoretical distribution was truncated with a cut-off by about 0,05 % v/v at both ends. The size class width was set according to a R20 series, which has a step ratio per class of $10^{1/20} = 1{,}122$ (see ISO 565).



Key

X distribution width, $D_{90,3}/D_{10,3}$

Y deviation, %

Figure C.1 — Influence of particle size distribution width on deviation of calculated size parameters

The data illustrate that conversions can be made having deviations smaller than 10 % from the theoretical values without truncation if the $D_{90,3}/D_{10,3}$ratio is smaller than about 3,5. Moreover Figure C.1 shows the increasing deviation for calculated particle size distribution parameters at increasing size distribution widths for values that are positioned near the end of the measured distribution (in this case the lower size end of the volume-based distribution). It also clearly shows that particle size distribution parameters having values in the middle part of the measured distribution, such as the $<D_{4,3}>$ and the $<D_{3,2}>$, have deviations smaller than 1 %. Note that all parameters were calculated to have less than 1 % bias without truncation of the distribution.

The influence of the size class width is also illustrated when the R5 series resolution (step width $10^{1/5}$ = 1,585) is used in the same lognormal distribution as above. For example, linear interpolation in the relevant size class leads here to a $D_{50,3}$ value of 5,132 µm (bias 2,6 %), whereas logarithmic interpolation gives the correct value of 5,0 µm. Of course, the method of interpolation depends on the set up of size classes for the distribution.

It can be concluded that the accuracy of calculated values for mean sizes and characteristic size parameters may be largely reduced by the conversion if

— the particle size distribution is wide,

— the distribution is truncated and

— the type of the distribution (dimensionality *r*) is changed considerably.

Thus, it is advised to check potential deviations through simulations, using e.g. Excel[2] sheets, in cases where high accuracy is required.

2) Excel is the trade name of a product supplied by Microsoft. This information is given for the convenience of users of this document and does not constitute an endorsement by ISO of the product named. Equivalent products may be used if they can be shown to lead to the same results.

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