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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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Foreword

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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-1} and x_i within the given size range of a distribution:

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

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

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, $q_0(x)$:

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

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):

$$\bar{x}_{1,0} = M_{1,0} \qquad (8)$$

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

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

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

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

4.2.3 Weighted mean particle sizes

Weighted mean particle sizes are defined by:

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

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:

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

