Designation: E2578 – 07

Standard Practice for
Calculation of Mean Sizes/Diameters and Standard Deviations of Particle Size Distributions[1]

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1. Scope

1.1 The purpose of this practice is to present procedures for calculating mean sizes and standard deviations of size distributions given as histogram data (see Practice E1617). The particle size is assumed to be the diameter of an equivalent sphere, e.g., equivalent (area/surface/volume/perimeter) diameter.

1.2 The mean sizes/diameters are defined according to the Moment-Ratio (M-R) definition system.[2,3,4]

1.3 This practice uses SI (Système International) units as standard.

1.4 *This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to use.*

2. Referenced Documents

2.1 *ASTM Standards:*[5]

E1617 Practice for Reporting Particle Size Characterization Data

3. Terminology

3.1 *Definitions of Terms Specific to This Standard:*

3.1.1 *diameter distribution*, *n*—the distribution by diameter of particles as a function of their size.

3.1.2 *equivalent diameter*, *n*—diameter of a circle or sphere which behaves like the observed particle relative to or deduced from a chosen property.

3.1.3 *geometric standard deviation*, *n*—exponential of the standard deviation of the distribution of log-transformed particle sizes.

3.1.4 *histogram*, *n*—a diagram of rectangular bars proportional in area to the frequency of particles within the particle size intervals of the bars.

3.1.5 *lognormal distribution*, *n*—a distribution of particle size, whose logarithm has a normal distribution; the left tail of a lognormal distribution has a steep slope on a linear size scale, whereas the right tail decreases gradually.

3.1.6 *mean particle size/diameter*, *n*—size or diameter of a hypothetical particle such that a population of particles having that size/diameter has, for a purpose involved, properties which are equal to those of a population of particles with different sizes/diameters and having that size/diameter as a mean size/diameter.

3.1.7 *moment of a distribution*, *n*—a moment is the mean value of a power of the particle sizes (the 3rd moment is proportional to the mean volume of the particles).

3.1.8 *normal distribution*, *n*—a distribution which is also known as Gaussian distribution and as bell-shaped curve because the graph of its probability density resembles a bell.

3.1.9 *number distribution*, *n*—the distribution by number of particles as a function of their size.

3.1.10 *order of mean diameter*, *n*—the sum of the subscripts p and q of the mean diameter $\overline{D}_{p,q}$.

3.1.11 *particle*, *n*—a discrete piece of matter.

3.1.12 *particle diameter/size*, *n*—some consistent measure of the spatial extent of a particle (see *equivalent diameter*).

3.1.13 *particle size distribution*, *n*—a description of the size and frequency of particles in a population.

3.1.14 *population*, *n*—a set of particles concerning which statistical inferences are to be drawn, based on a representative sample taken from the population.

3.1.15 *sample*, *n*—a part of a population of particles.

3.1.16 *standard deviation*, *n*—most widely used measure of the width of a frequency distribution.

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[1] This practice is under the jurisdiction of ASTM Committee E56 on Nanotechnology and is the direct responsibility of Subcommittee E56.02 on Characterization: Physical, Chemical, and Toxicological Properties.

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[2] Alderliesten, M., "Mean Particle Diameters. Part I: Evaluation of Definition Systems," *Part. Part. Syst. Charact.*, 7, 1990, pp. 233-241.

[3] Alderliesten, M., "Mean Particle Diameters. From Statistical Definition to Physical Understanding," *J. Biopharm.Statist.*, 15, 2005, pp. 295-325.

[4] Mugele, R. A., Evans, H. D., "Droplet Size Distribution in Sprays," *Ind. Eng. Chem.*, 43, 1951, pp. 1317-1324.

[5] For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.

3.1.17 *surface distribution*, *n*—the distribution by surface area of particles as a function of their size.

3.1.18 *variance*, *n*—a measure of spread around the mean; square of the standard deviation.

3.1.19 *volume distribution*, *n*—the distribution by volume of particles as a function of their size.

4. Summary of Practice

4.1 Samples of particles to be measured should be representative for the population of particles.

4.2 The ‘frequency’ of a particular value of a particle size D can be measured (or expressed) in terms of the number of particles, the cumulated diameters, surfaces or volumes of the particles. The corresponding frequency distributions are called Number, Diameter, Surface, or Volume distributions.

4.3 As class mid points D_i of the histogram intervals the arithmetic mean values of the class boundaries are used.

4.4 Particle shape factors are not taken into account, although their importance in particle size analysis is beyond doubt.

4.5 A coherent nomenclature system is presented which conveys the physical meanings of mean particle diameters.

5. Significance and Use

5.1 Mean particle diameters defined according to the Moment-Ratio (M-R) system are derived from ratios between two moments of a particle size distribution.

6. Mean Particle Sizes/Diameters

6.1 *Moments of Distributions*:

6.1.1 Moments are the basis for defining mean sizes and standard deviations. A random sample, containing N elements from a population of particle sizes D_i, enables estimation of the moments of the size distribution of the population of particle sizes. The r-th sample moment, denoted by M_r', is defined to be:

$$M_r' := N^{-1}\sum_i n_i D_i^r \tag{1}$$

where $N = \sum_i n_i$, D_i is the midpoint of the i-th interval and n_i is the number of particles in the i-th size class (i.e., class frequency). The (arithmetic) sample mean M_1' of the particle size D is mostly represented by $\bar{D}$. The r-th sample moment about the mean $\bar{D}$, denoted by M_r, is defined by:

$$M_r := N^{-1}\sum_i n_i (D_i - \bar{D})^r \tag{2}$$

6.1.2 The best-known example is the sample variance M_2. This M_2 always underestimates the population variance σ_D^2 (squared standard deviation). Instead, M_2 multiplied by $N/(N-1)$ is used, which yields an unbiased estimator, s_D^2, for the population variance. Thus, the sample variance s_D^2 has to be calculated from the equation:

$$s_D^2 = \frac{N}{N-1}M_2 = \frac{\sum_i n_i (D_i - \bar{D})^2}{N-1} \tag{3}$$

6.1.3 Its square root is the standard deviation s_D of the sample (see also 6.3). If the particle sizes D are lognormally distributed, then the logarithm of D, ln$D$, follows a normal distribution (Gaussian distribution). The geometric mean $\bar{D}_g$ of the particle sizes D equals the exponential of the (arithmetic) mean of the (ln$D$)-values:

$$\bar{D}_g = \exp[N^{-1}\sum_i n_i (\ln D_i)] = \sqrt[N]{\prod_i D_i^{n_i}} \tag{4}$$

6.1.4 The standard deviation $s_{\ln D}$ of the (ln$D$)-values can be expressed as:

$$s_{\ln D} = \sqrt{\frac{\sum_i n_i \{\ln(D_i/\bar{D}_g)\}^2}{N-1}} \tag{5}$$

6.2 *Definition of Mean Diameters* $\bar{D}_{p,q}$:

6.2.1 The mean diameter $\bar{D}_{p,q}$ of a sample of particle sizes is defined as $1/(p - q)$-th power of the ratio of the p-th and the q-th moment of the Number distribution of the particle sizes:

$$\bar{D}_{p,q} = \left[\frac{M_p'}{M_q'}\right]^{1/(p-q)} \qquad \text{if } p \neq q \tag{6}$$

6.2.2 Using Eq 1, Eq 6 can be rewritten as:

$$\bar{D}_{p,q} = \left[\frac{\sum_i n_i D_i^p}{\sum_i n_i D_i^q}\right]^{1/(p-q)} \qquad \text{if } p \neq q \tag{7}$$

6.2.3 The powers p and q may have any real value. For equal values of p and q it is possible to derive from Eq 7 that:

$$\bar{D}_{q,q} = \exp\left[\frac{\sum_i n_i D_i^q \ln D_i}{\sum_i n_i D_i^q}\right] \qquad \text{if } p = q \tag{8}$$

6.2.4 If $q = 0$, then:

$$\bar{D}_{0,0} = \exp\left[\frac{\sum_i n_i \ln D_i}{\sum_i n_i}\right] = \sqrt[N]{\prod_i D_i^{n_i}} \tag{9}$$

6.2.5 $\bar{D}_{0,0}$ is the well-known geometric mean diameter. The physical dimension of any $\bar{D}_{p,q}$ is equal to that of D itself.

6.2.6 Mean diameters $\bar{D}_{p,q}$ of a sample can be estimated from any size distribution $f_r(D)$ according to equations similar to Eq 7 and 8:

$$\bar{D}_{p,q} = \left[\frac{\sum_i^m f_r(D_i) D_i^{p-r}}{\sum_i^m f_r(D_i) D_i^{q-r}}\right]^{1/p-q} \qquad \text{if } p \neq q \tag{10}$$

and:

$$\bar{D}_{p,p} = \exp\left[\frac{\sum_i^m f_r(D_i) D_i^{p-r} \ln D_i}{\sum_i^m f_r(D_i) D_i^{p-r}}\right] \qquad \text{if } p = q \tag{11}$$

where:

$f_r\,(D_i)$ = particle quantity in the i-th class,

D_i = midpoint of the i-th class interval,

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

m = number of classes.

6.2.7 If $r = 0$ and we put $n_i = f_0(D_i)$, then Eq 10 reduces to the familiar form Eq 7.

TABLE 1 Nomenclature for Mean Particle Diameters $\overline{D}_{p,q}$

Systematic Code	Nomenclature
$\overline{D}_{-3.0}$	harmonic mean volume diameter
$\overline{D}_{-2.1}$	diameter-weighted harmonic mean volume diameter
$\overline{D}_{-1.2}$	surface-weighted harmonic mean volume diameter
$\overline{D}_{-2.0}$	harmonic mean surface diameter
$\overline{D}_{-1.1}$	diameter-weighted harmonic mean surface diameter
$\overline{D}_{-1.0}$	harmonic mean diameter
$\overline{D}_{0.0}$	geometric mean diameter
$\overline{D}_{1.1}$	diameter-weighted geometric mean diameter
$\overline{D}_{2.2}$	surface-weighted geometric mean diameter
$\overline{D}_{3.3}$	volume-weighted geometric mean diameter
$\overline{D}_{1.0}$	arithmetic mean diameter
$\overline{D}_{2.1}$	diameter-weighted mean diameter
$\overline{D}_{3.2}$	surface-weighted mean diameter
$\overline{D}_{4.3}$	volume-weighted mean diameter
$\overline{D}_{2.0}$	mean surface diameter
$\overline{D}_{3.1}$	diameter-weighted mean surface diameter
$\overline{D}_{4.2}$	surface-weighted mean surface diameter
$\overline{D}_{5.3}$	volume-weighted mean surface diameter
$\overline{D}_{3.0}$	mean volume diameter
$\overline{D}_{4.1}$	diameter-weighted mean volume diameter
$\overline{D}_{5.2}$	surface-weighted mean volume diameter
$\overline{D}_{6.3}$	volume-weighted mean volume diameter

6.3 *Standard Deviation*:

6.3.1 According to Eq 3, the standard deviation of the Number distribution of a sample of particle sizes can be estimated from:

$$s_D = \sqrt{\frac{\sum_i n_i D_i^2 - N\overline{D}_{1,0}^2}{N-1}} \tag{12}$$

which can be rewritten as:

$$s = c\sqrt{\overline{D}_{2,0}^2 - \overline{D}_{1,0}^2} \tag{13}$$

with:

$$c = \sqrt{N/(N-1)} \tag{14}$$

6.3.2 In practice, $N >> 100$, so that $c \approx 1$. Hence:

$$s \approx \sqrt{\overline{D}_{2,0}^2 - \overline{D}_{1,0}^2} \tag{15}$$

6.3.3 The standard deviation $s_{\ln D}$ of a lognormal Number distribution of particle sizes D can be estimated by (see Eq 12):

$$s_{\ln D} = \sqrt{\frac{\sum_i n_i \{\ln(D_i/\overline{D}_{0,0})\}^2}{N-1}} \tag{16}$$

6.3.4 In particle-size analysis, the quantity s_g is referred to as the geometric standard deviation[2] although it is not a standard deviation in its true sense:

$$s_g = \exp[s_{\ln D}] \tag{17}$$

6.4 *Relationships Between Mean Diameters* $\overline{D}_{p,q}$:

6.4.1 It can be shown that:

$$\overline{D}_{p,0} \leq \overline{D}_{m,0} \qquad \text{if } p \leq m \tag{18}$$

and that:

$$\overline{D}_{p-1,\,q-1} \leq \overline{D}_{p,q} \tag{19}$$

6.4.2 Differences between mean diameters decrease according as the uniformity of the particle sizes D increases. The equal sign applies when all particles are of the same size. Thus, the differences between the values of the mean diameters provide already an indication of the dispersion of the particle sizes.

6.4.3 Another relationship very useful for relating several mean particle diameters has the form:

$$[\overline{D}_{p,q}]^{p-q} = \overline{D}_{p,0}^p / \overline{D}_{q,0}^q \tag{20}$$

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

6.4.5 Eq 20 is particularly useful when a specific mean diameter cannot be measured directly. Its value may be calculated from two other, but measurable mean diameters.

6.4.6 Eq 7 also shows that:

$$\overline{D}_{p,q} = \overline{D}_{q,p} \tag{21}$$

6.4.7 This simple symmetry relationship plays an important role in the use of $\overline{D}_{p,q}$.

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

$$O = p + q \tag{22}$$

6.4.9 For lognormal particle-size distributions, there exists a very important relationship between mean diameters:

$$\overline{D}_{p,q} = \overline{D}_{0,0}\exp[(p+q)s_{\ln D}^2/2] \tag{23}$$

6.4.10 Eq 23 is a good approximation for a sample if the number of particles in the sample is large ($N > 500$), the standard deviation $\sigma_{\ln D} < 0.7$ and the order O of $\overline{D}_{p,q}$ not larger than 10. Erroneous results will be obtained if these requirements are not fulfilled. For lognormal particle-size distributions, the values of the mean diameters of the same order are equal. Conversely, an equality between the values of these mean diameters points to lognormality of a particle-size distribution. For this type of distribution a mean diameter $\overline{D}_{p,q}$ can be rewritten as $\overline{D}_{j,j}$, where $j = (p + q)/2 = O/2$, if O is even.

6.4.11 Sample calculations of mean particle diameters and (geometric) standard deviation are presented in Appendix X1.

7. Nomenclature of Mean Particle Sizes/Diameters[6]

7.1 Table 1 presents the M-R nomenclature of mean diameters, an unambiguous list without redundancy. This nomenclature conveys the physical meanings of mean particle diameters.

7.2 The mean diameter $\overline{D}_{3.2}$ (also called: Sauter-diameter) is inversely proportional to the volume specific surface area.

8. Keywords

8.1 distribution; equivalent size; mass distribution; mean particle size; mean particle diameter; moment; particle size; size distribution; surface distribution; volume distribution

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[6] Alderliesten, M., "Mean Particle Diameters. Part II: Standardization of Nomenclature," *Part. Part. Syst. Charact.*, 8, 1991, pp. 237-241.