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Mono-Size Distribution Index (*MSDI*): A new criterion for the quantitative description of size distribution

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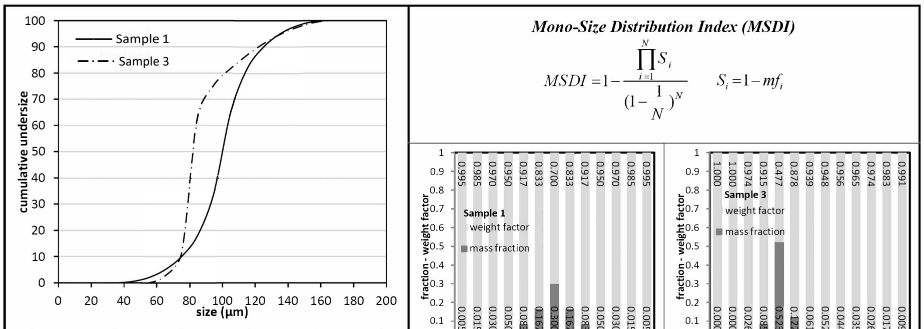
HIGHLIGHTS

- Quantitative description of particle size distribution (PSD).
- Drawback of previous descriptive parameters of PSD.
- Propose a new parameter named mono-size distribution index (*MSDI*).

GRAPHICAL ABSTRACT



	D_{10}	D_{50}	D_{90}	*SPAN*
Sample 1	65	100	125	0.6
Sample 3	65	82	122	0.695

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ABSTRACT

Graphical size distribution is widely used in different fields of science and studies related to powders, droplets, bubbles, and pores. However, in some condition it may also be necessary to express the size distribution quantitatively. In spite of there being several suggested ways to quantify size distribution in the literature, some of these approaches are not applicable for many methods and the rest have other drawbacks. In this study, first, some quantitative size distribution methods (such as the polydispersity index) and their defects are concisely discussed. *SPAN* seems to be the most generally appropriate method, its parameters are determined from cumulative size distribution data. Nevertheless, some specific results imply that there are still some drawbacks in this method. Next, a new quantitative description of size distribution is presented which is applicable to many different techniques. In this method the characterization value is limited to 0 and 1, where 0 is related to completely polydispersed size distribution and 1 denotes the completely monodispersed size distribution.

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1. Introduction

Powders, pores, droplets, bubbles, and so on (in generally particles) are widely used in many different systems. Particle size distribution has a significant effect on the overall efficiency of the processes that deal with particles. Therefore, controlling the size of particles is the subject of various scientific investigations. There is a vast usage of graphical presentation of size distribution in the literature. Particle size distribution (PSD) graphs can give a clear view of the particles size dispersion of a sample. Nevertheless, comparison of the particle size of different samples is usually difficult when the difference between PSD curves is small. In this case, PSD is often presented quantitatively, especially when production of mono-sized particles is the main aim of a study. Furthermore, PSD information could be presented more concisely using descriptive parameters of particle size distribution.

Different quantitative size distribution parameters are used by researchers are often referred to as polydispersity or monodispersity. It should be noted that in polymer science the term polydispersity, which is defined as the weight average divided by the number of average molecular weight (M_w/M_n) [1], is different from what is referred to in this paper. Mikuska et al. considered the geometric standard deviation as the monodispersity criterion of aerosol particles [2]. Lower values of geometric standard deviation are related to more uniform PSD (for monodisperse particles this factor is less than 1.25) [3]. Gao et al. used the standard deviation of the particles diameter divided by the mean diameter as the monodispersity index. A sample is called monodispersed if the value of this index is less than 5% [4]. Yu *et al.* investigated the size distribution of produced polymer particles in the annealing process of polystyrene (PS)/poly(methyl methacrylate) (PMMA) blends [5]. They reported that the final properties of the product depended not only on the mean size of the polymer particles but also on its size distribution. They suggested the ratio of volume average diameter (d_v) per number average diameter (d_n) as the polydispersity index as shown in Eq. (1).

$$PI = \frac{d_v}{d_n} \tag{1}$$

where:

$$d_n = \frac{\sum_{i=1}^{n} d_i}{n} \tag{2}$$

$$d_v = \sqrt[3]{\frac{6\sum_{i=1}^{n} v_i}{\pi n}} \tag{3}$$

In these relationships, d_i and v_i are equivalent diameter and particle volume for each cut, respectively. For monodispersed particles, $d_n = d_v$, therefore, $PI = 1$. On the other hand, the polydispersity index is greater than one for non-monodispersed size distributions [5].

Coefficient of variation (C_v) of particles diameter as a criterion of monodispersity was used in the study of Ha *et al.* [6]. They determined the diameter of particles (of at least 100 individual particles) using SEM images and C_v was calculated using the Eq. (4).

$$C_v = 100 \times \left\{ \left(\sum (d_i - d_n)^2 / n\right)^{0.5} / d_n \right\} \tag{4}$$

They reported that highly monodisperse polystyrene particles have a coefficient of variation of about 1%.

Size and size distribution of nanopowders can be estimated using the dynamic light scattering (DLS) measurement system. In this technique, the polydispersity index is obtained according to photon correlation spectroscopic analysis. It is extrapolated from the autocorrelation function and varies between 0.01 for mono dispersed particles up to 0.5-0.7 for samples with broad size distribution [7-9]. The polydispersity index is calculated using a computer program in this technique. In the DLS technique a few large particles in a mixture (which scatter more light than smaller ones) can produce misleading results (such as underestimation of the amount of small particles) [10,11]. In addition, the DLS technique is applicable only for submicron size particles.

Size distribution has been investigated in a considerable number of studies using D_{10}, D_{50}, and D_{90}. These parameters were obtained from cumulative size distribution. Also, the distribution ratio (D_{90}/D_{10}) has been used in the work of different researchers [12,13], where its higher value indicates a much broader PSD. In other surveys, the width of the particle size distribution (known as *SPAN* in the literature) has been used as a quantitative PSD criterion [14-16]. *SPAN* can be calculated using Eq. (5). A lower value of this parameter denotes a uniform PSD.

$$SPAN = \frac{D_{90} - D_{10}}{D_{50}} \tag{5}$$

2. Drawback of previous methods

Quantifying of particle size distribution would lead to a more concise and precise comparison, especially when there is only a small difference between PSD curves. Although, there are several methods for expressing the particle size distribution quantitatively, some of these methods parameters cannot be determined or calculated (simply or straightly) for any sample. In other words, these methods are limited to some especial samples. In addition, the value of these criteria is borderless (e.g. are not limited to the values of zero and one).

SPAN may be a suitable method, as it is easily applicable to any sample. It just uses D_{10}, D_{50}, and D_{90}, which are simply determined from cumulative size distribution data. However, Torrecillas *et al.* showed that a significant error would be introduced if the PSD curves have different peaks on both sides of the mean diameter. In their experiment a sample with d_{10}= 92.27, d_{50}= 562.7, and d_{90}= 971.9 and another sample with d_{10}= 143.5, d_{50}= 677.2, and d_{90}= 1218 have a *SPAN* of 1.563 and 1.587, respectively [17]. According to their results, two different particle samples with completely different PSD have almost the same *SPAN* value. In addition to the work of Torrecillas, it is possible that samples with different particle size distributions have the same *SPAN*, if their D_{10}, D_{50}, and D_{90} values are identical. Therefore, it seems that this is an unreliable definition in some conditions. Consider the typical differential size distribution of two different samples as shown in Fig 1.

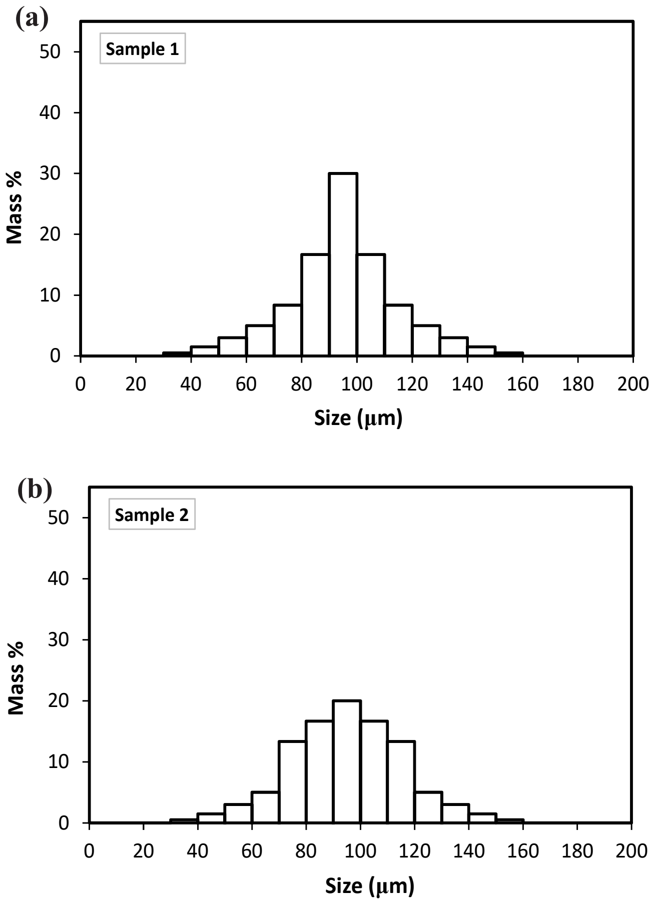

Fig. 1. Typical differential size distribution histograms of two different samples. (a) Sample 1 with more uniform particle size distribution. (b) Sample 2 with broader particle size distribution.

As seen in Fig. 1, the PSD of sample 2 is obviously broader than the PSD of sample 1. The cumulative under size distribution curves of these samples are presented in Fig. 2. Although the size distributions of these two samples are different, Fig. 2 reveals that the values of D_{10}, D_{50}, and D_{90} of the both samples are the same, leading to identical values for their *SPAN*.

In general, the lower values of *SPAN* indicate more uniformity in the size distribution. Nevertheless, in some cases, it is probable that a powder with narrower PSD has a greater value of *SPAN* than a powder with broader particle size distribution. This situation is shown in Figs. 3 and 4, where a typical differential and cumulative PSD of two different samples are presented, respectively

It is clearly seen in Fig. 3, sample 3 has a narrower size distribution than sample 1. Nevertheless, the values of *SPAN* for these samples, obtained from the data of Fig. 4, represent the opposite result. The values of D_{10}, D_{50}, and D_{90} and *SPAN* of each sample are reported in Table 1.

The results in Table 1 reveal that although sample 3 has a narrower size distribution it has a greater value of *SPAN*.

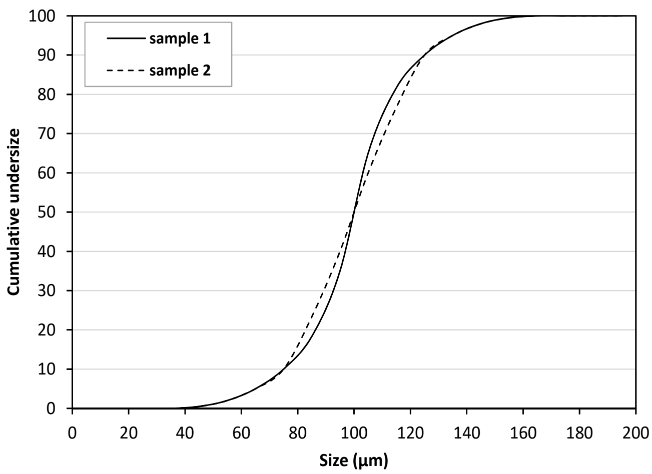

Fig. 2. Cumulative under size distribution curves of typical samples 1 and 2.

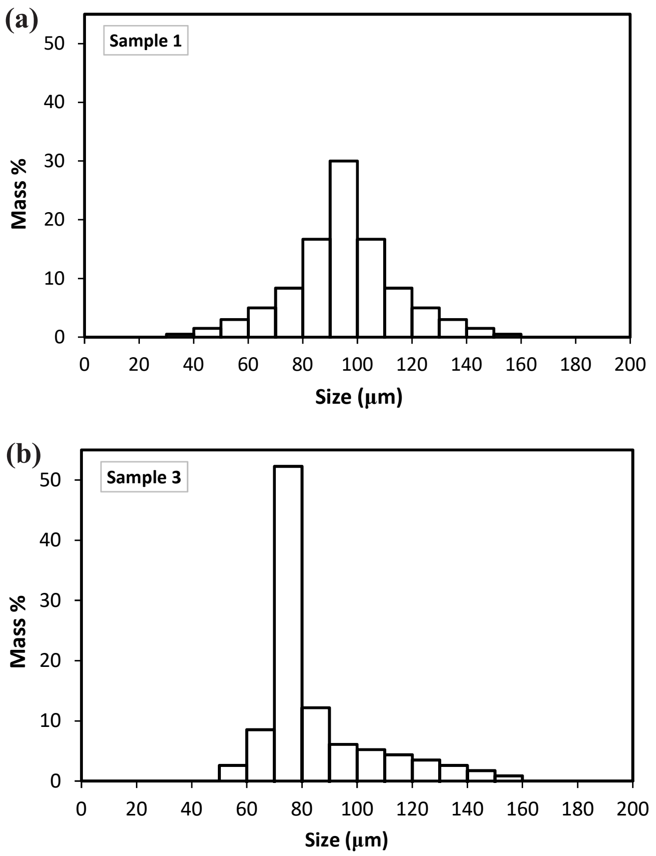

Fig. 3. Typical differential size distribution histograms of two different samples. (a) Sample 1 with broader particle size distribution. (b) Sample 3 with narrower particle size distribution.

In addition to the mentioned drawbacks of *SPAN*, its value is not limited between zero and one. In other words, polydispersed powder may have a value of SPAN greater than one (*SPAN* of one is not related to the completely polydispersed powder).

Therefore, it is necessary to define a new quantitative description of PSD, which will resolve the above mentioned problems.

3. Mono-Size Distribution Index (*MSDI*)

In this paper, a new quantitative description of PSD is defined in such a way that its value was limited between zero and one. The value of zero represents the completely polydispersed sample (i.e. the same percent in each size interval), and the value of one shows the

Table 1. Values of D_{10}, D_{50}, D_{90}, and SPAN of typical samples 1 and 3.

Sample	D_{10}	D_{50}	D_{90}	*SPAN*
1	65	100	125	0.6
3	65	82	122	0.695

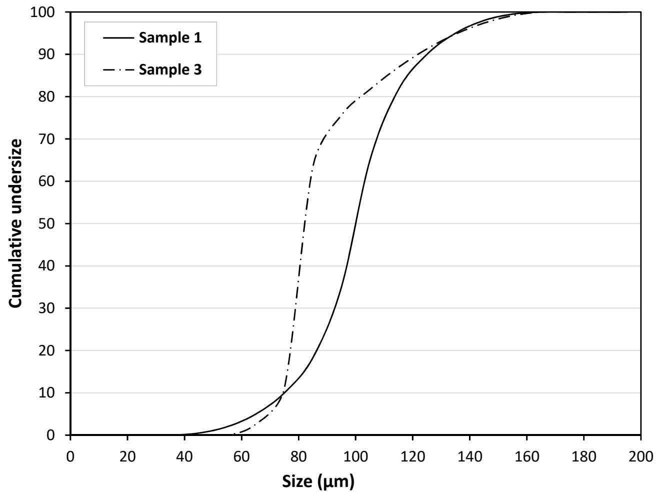

Fig. 4. Cumulative under size distribution curves of typical samples 1 and 3.

completely monodispersed sample (i.e. particles place on one size interval). Generally, each size interval has a weight factor that depends on the fraction of particle on it. This fraction can be mass base, number base, etc. This new criterion is called the Mono-Size Distribution Index (*MSDI*), and is presented by Eq. (6) and complementary Eq. (7).

$$MSDI = 1 - \frac{\prod_{i=1}^{N} S_i}{(1-\frac{1}{N})^N} \tag{6}$$

$$S_i = 1 - mf_i \tag{7}$$

where N, S_i and mf_i are the total number of size interval, weight factor, and fraction of i^{th} size interval, respectively. According to Eq. (6) and data in Fig. 5, the *MSDI* of sample 1, sample 2, and sample 3 are calculated as 0.057, 0.037, and 0.176, respectively.

Obtained results of this study show that *MSDI* correctly differs between sample 1 and sample 2. The value of *MSDI* for sample 2 is lower than sample 1, representing the broader size distribution of sample 2 (whereas the *SPAN* of these samples are the same). In addition, the *MSDI* of sample 3 is greater than sample 1, which indicates that sample 3 has a narrower size distribution of compared with sample 1 (whereas *SPAN* quantifies the PSD of these sample incorrectly).

4. Conclusion

There are different methods in the literature that quantify the particle size distribution of powders, pores,

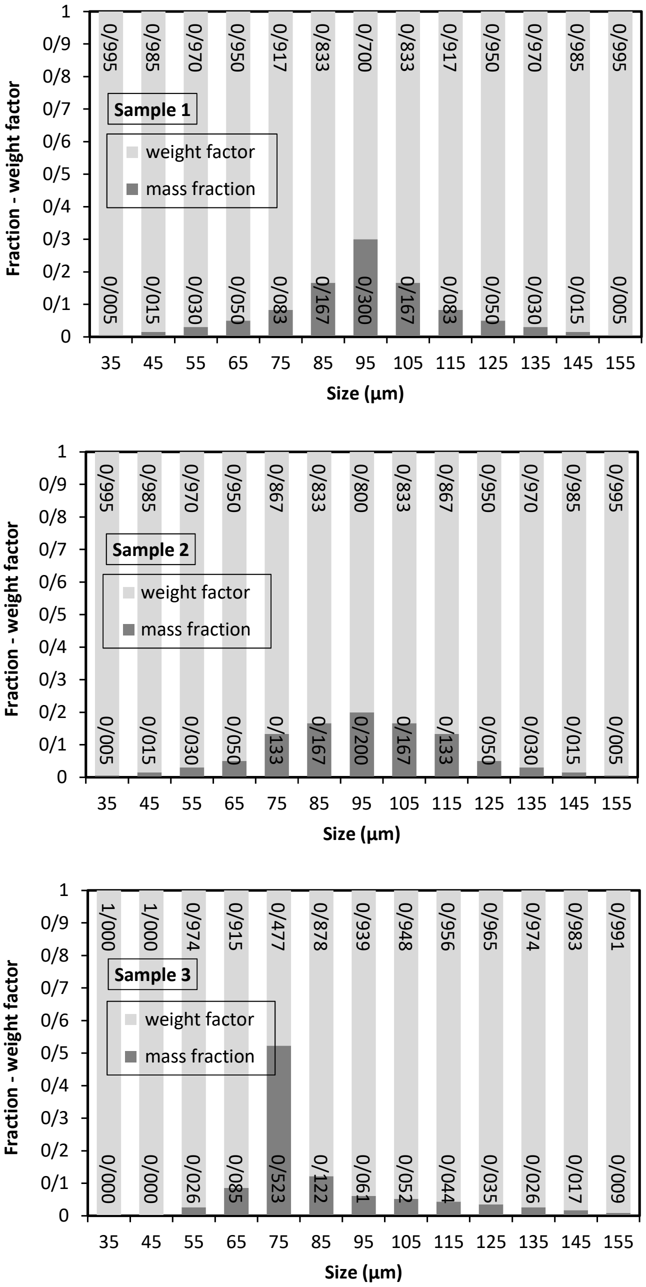

Fig. 5. Fraction and weight factor of each size interval for different typical samples used in this study.

droplets, bubble, and so on. However, some methods are limited to a specific size range. For example, although the polydispersity index can be easily determine using a computer program in the dynamic light scattering (DLS) measurement system, this technique is limited to the submicron particle size. In other methods, various statistical parameters (such as the geometric standard deviation, coefficient of variation, etc.) are suggested as monodispersity or polydispersity index. The fact that these indexes are not limited to two values is the biggest drawback of these methods. *SPAN* may be a suitable quantitative PSD criterion because it does not have the mentioned drawbacks. However, as shown in this paper, *SPAN* also has its own defects. First, if different powders have the same D_{10}, D_{50}, and D_{90} they will have identical *SPAN* values. Second, greater *SPAN* values from narrower size distribution data (a contradictory result) may occur in some conditions. (In general, lower values of *SPAN* indicate more uniformity in size distribution). The Mono-size distribution index (*MSDI*), as a new criterion presented in this work, solved these deficiencies. The *MSDI* can be easily applicable for any particle sample. According to its mathematical formula (Eqs. (6) and (7)), it only needs size distribution data. Its value is limited to zero and one. The value of zero represents a completely polydispersed sample and the value of one shows a completely monodispersed sample. In addition, *MSDI* quantify the PSD data of three typical samples presented in this paper correctly, where the *SPAN* presents illusory results.

References

[1] M. Ji, H. Liu, X. Yang, Synthesis of monodisperse SiO_2/P(DVB-SO_3H)/SiO_2/P(DVB-SO_3H) tetra-layer polyelectrolyte microspheres and the corresponding hollow P(DVB-SO_3H) polyelectrolyte microspheres with a shell-in-shell structure, Polym. Chem. 2 (2010) 148-156.

[2] P. Mikuška, L. Čapka, Z. Večeřa, Aerosol sampler for analysis of fine and ultrafine aerosols, Anal. Chim. Acta, 1020 (2018) 123-133.

[3] D.A. Japuntich, J.I.T. Stenhouse, B.Y.H. Liu, Conditions for monodispersity of heterogeneous condensation aerosols using dimensionless groups, J. Colloid Interf. Sci. 136 (1990) 393-400.

[4] C. Gao, X. Qi, Z. Zhang, S. Chen, B. Li, W. Huang, Fabrication of monodisperse precursor gel microspheres for hollow glass microspheres by combining the sol-microemulsion-gel process with a T-shaped microfluidic device, Int. J. Hydrogen Energ. 36 (2011) 9758-9766.

[5] W. Yu, C. Zhou, T. Inoue, A coalescence mechanism for the coarsening behavior of polymer blends during a quiescent annealing process. II. Polydispersed particle system, J. Polym. Sci. Pol. Phys. 38 (2000) 2390-2399.

[6] S.T. Ha, O.O. Park, Size control of highly monodisperse polystyrene particles by modified dispersion polymerization. J. Macromol. Res. 18

(2010) 935-943.

[7] V. Jain, P. Kare, D. Jain, R. Singh, Development and characterization of mucoadhesive nanosuspension of ciprofloxacin, Acta Pol. Pharm. 68 (2011) 273-278.

[8] B. Anilreddy, Preparation and characterization of iron oxide nanoparticles on disaccharide templates, Asian JPRHC, 1 (2009) 172-183.

[9] N. Tresilwised, P. Pithayanukul, C. Plank, Factors affecting sizes of magnetic particles formed by chemical co-precipitation. J. Pharm. Sci. 32 (2005) 71-76.

[10] K. Mehrabi, B. Nowack, Y.A.R. Dasilva, D.M. Mitrano, Improvements in nanoparticle tracking analysis to measure particle aggregation and mass distribution: A case study on engineered nanomaterial stability in incineration landfill leachates, Environ. Sci. Technol. 51 (2017) 5611-5621.

[11] J. Hou, H. Ci, P. Wang, C. Wang, B. Lv, L. Miao, G. You, Nanoparticle tracking analysis versus dynamic light scattering: Case study on the effect of Ca^{2+} and alginate on the aggregation of cerium oxide nanoparticles, J. Hazard. Mater. 360 (2018) 319-328.

[12] M.G. Rasteiro, A. Tomas, L. Ferreira, S. Figueiredo, PVC paste rheology: Study of process dependencies. J. Appl. Polym. Sci. 112 (2009) 2809-282.

[13] V.K. Langsi, B. A. Ashu-Arrah, N. Ward, J.D. Glennon, Synthesis and characterisation of non-bonded 1.7 μm thin-shell (TS1.7-100 nm) silica particles for the rapid separation and analysis of uric acid and creatinine in human urine by hydrophilic interaction chromatography, J. Chromatogr. A, 1506 (2017) 37-44.

[14] M. Velez1, Y. He1, D.E. Day, T.P. Schuman, K.V. Kilway, J.R. Melander, R.A. Weiler, B.D. Miller, E.L. Nalvarte, J.D. Eick, Processing of yttrium aluminosilicate (YAS) glasses for dental composites, Cerâmica, 57 (2011) 1-9.

[15] A. Tascón, Influence of particle size distribution skewness on dust explosibility, Powder Technol. 338 (2018) 438-445.

[16] M. Ghasemi, P. Alexandridis, M. Tsianou, Conversion of particle size distribution data from mass to number-based and its application to biomass processing, Biosyst. Eng. 176 (2018) 73-87.

[17] C.M. Torrecillas, G.W. Halbert, D.A. Lamprou, A novel methodology to study polymodal particle size distributions produced during continuous wet granulation, Int. J. Pharm. 519 (2017) 230-239.