Particle size distributions in Earth Sciences: a review of techniques and a new procedure to match 2D and 3D analyses

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Review

In the abstract, the authors announce that: "Here, we (1) present a critical review of most commonly used techniques to calculate particle size distributions from cohesive and loose samples, and (2) we illustrate a new calculation formula to extract reliable 3D grain size distributions from 2D datasets", suggesting that: "Our promising results encourage the usage of Dw formula as it provides best matching results with 3D laser granulometry and needs basic input parameters that can be easily extracted from any image analysis software."

However, title and abstract are misleading. The "review of techniques of most commonly used techniques" is strongly biased towards particle size analysis of loose samples as performed in sedimentology and does not do justice to other fields of Earth, Material or Engineering Sciences, where it is more common to analyze 2D sections of solid samples. The proposed "calculation formula" is neither new nor reliable, nor can the "Dw formula" be "easily" obtained from image analysis software. Most importantly, there is no need to develop a "new calculation formula to extract reliable 3D grain size distributions from 2D datasets" because it is simply not true that "nowadays there is no univocal correlation function linking particle size data from 2D image analysis to the corresponding 3D grain size distributions".

The paper is well written – if too long – but it cannot be published in its present form

Here is why:

... the paper is too long:

In the introduction to the review, it would have been sufficient to state that grain size analysis is important in almost all fields of the natural sciences. The entire section 1.1 (almost 4 pages) could be scratched because mentioning 110 publications that in some way or other deal with particle size analysis, without addressing their contents, damages rather than improves the paper. Most of these 'empty citations' are not referred to again in the rest of the paper, they simply blow up the reference list in an inflationary way to a total length of 196 entries. An – in this day and age – one has to make doubly sure not to write a text that reads as if AI had produced it.

A petrographic-mineralogical sample description is not necessary. The information given in section 5.1 (approx. 3 pages) is irrelevant in the context of this paper because the influence of petrographic-mineralogical details on the accuracy of the new method of particle size analysis is not discussed anywhere else in the paper. This whole section could be scratched too.

Figure 9 in section 5.2 shows the grain size distribution curves obtained by laser granulometer analysis. This figure is highly informative and clearly labeled. A description of what is shown in the figure (3 pages) is not necessary. This is a paper – not a talk. The same applies to the text that describe figure 12 which shows grain size distribution curves extracted from 2D thin sections through image analysis (3 more pages). What is important to know about these two figures is very nicely represented in figure 13, which shows a comparison of grain size distributions obtained from image analysis technique applied to thin sections, and the text that discusses it.

... the review is not satisfying:

In section 1.1, the authors write, that "particle size is defined as a scalar property of granular media and is typically calculated as the nominal diameter of particles ...". Now, the value of this "nominal" diameter depends very much on how it is measured and how it is defined. As different measures of central tendency, such as the arithmetic mean, the geometric mean, etc., as well as median or mode, in general, return different values for one and the same distribution. Mean values also come out differently, depending on whether the distribution is linear or logarithmic, and whether the data is weighted in one way or another.

Therefore, in section 1.2, it would have been important to discuss which type of input data was used by the different methods (weighted or non-weighted frequencies, linear or logarithmic bins, etc.), and how the "nominal diameter" was defined. Instead, it becomes apparent that the review presents a comparison of equipment and procedures suited for the analysis of sedimentological/granular samples. In the first part (until line 204), the focus is on the direct analysis of 3D particles, dealing mainly with sieving and particle analyzers. It is an evaluation of the use and the limitations of techniques of the different methods with Figure 1 presenting a very nice overview. Unfortunately, nothing is said about the mathematical basis of the data treatment, i.e., about how particle size distributions are "calculated" and how the "nominal diameter" is defined (which is what one would expect of a "critical" review). In the second part (lines 205ff), the focus is on analyzing 2D sections. This part is not very well researched and ends with profound errors and misconceptions.

... the new method is not new:

In the paper, the book by Heilbronner&Barrett (2014) is cited repeatedly, for example, in the context of "bi-dimensional automated-manual image analysis", "manual-automatic identification", or large sample size being necessary and time and labour involved for manual digitization. The authors obviously missed chapter 12 of this book which is entirely devoted to "3D Grain Size". In this chapter, a procedure is presented by which a unique parent population of spheres can be calculated from a given histogram of sectional circles. The program is called stripstar. Apart from calculating the distribution of 3D spheres, it also provides a test (using a purely mathematical concept of antispheres) which allows one to determine whether a given distribution of circles has a parent population of 3D spheres or not. The original code was written in Fortran. But for those who do not wish to use Fortran, the corresponding macro for ImageJ is readily available at https://github.com/kilir/Jazy_macros. In other words, it is possible and quite easy to convert a histogram of 2D circles to a histogram of the corresponding 3D spheres from which various types of mean, mode, median etc. can easily be calculated. For reasons of physical significance, it is argued in this chapter to use the mode, not the arithmetic mean, of the volume weighted size distribution of 3D spheres. – Please note that the stripstar method is by no means the first of its kind. Methods for calculating size distributions of spheres from section diameters have been developed already 100 years ago. Early attempts are by Wicksell (1923 and 1925) in anatomy, later by Saltikov (1958) in metallurgy and many others. An excellent overview of such pre-computer-age stereological methods is given by Underwood (1979). First versions of stripstar, using a different mathematical approach, were written in the 1990's, when computers were readily available.

The same chapter 12 also discusses the use and the limitations of so-called shortcuts. One of them consists of volume weighting the distribution of 2D sectional circles. It is demonstrated that this short cut can only approximate but not reproduce the true (stripstar-calculated) distribution of 3D spheres. Thus, the arithmetic mean for such shortcut-distributions would not reliably reproduce the true value. Now, volume-weighting is exactly what is introduced in this paper as a "new calculation formula". Except that, here, it is proposed to additionally correct the volume-weighted distribution by taking into consideration the average shape of the grains. Even though the shape factor (so-called surface area correction, Fig.15) is clearly dependent on particle aspect ratio and size, a constant average value is used for each sample. Why? It would be easy – and more physically meaningful – to take the shape factor into account for each grain individually. Otherwise it might be seen as just one more fudge factor to make the 2D mean equal to the 3D mean.

... the development and test of the "new Dw formula" is not rigorous:

The approach taken by the authors for creating and testing this new method cannot succeed. Even if the "new Dw formula" were a good idea, one cannot use natural samples with an unknown size distribution and the measurements provided by a specific particle analyzer to check if the the formula derives the correct results from 2D sections. When creating and testing a new procedure for converting 2D to 3D grain size data, it is paramount to use standard test samples, made from glass beads, for example, with an excatly known size distribution. It is important to exclude the effect of shape or composition because both particle analyzers and image analysis are susceptible, in different ways, to the naturally occurring deviations from constant shape and composition. Moreover, both particle analyzer and image analysis results have to be matched against the exactly known data of the standard sample.

It is well known that particle analyzers, even with the most careful sample preparation, are prone to producing inconsistent results, from analyzer to analyzer, from sample to sample, from run to run. A lot depends on the software packages used to operate them, and the specific settings selected for a given run. In contrast, image analysis methods only depend on the geometry of the particles, not on the composition and physical behaviour during analysis. With this in mind, one might even argue that image analysis plus 2D-3D conversion (stripstar) comes closer to the true distribution of particles than results from particle analyzers.

... I recommend re-writing the paper:

For the reasons given above, the submitted paper should not be published. But it would be a pity if those excellent data sets, which have been created with a lot of effort, would go to waste. I assume that the original incentive for developing this Dw calculation was to be able to process a large number of different sands for research or engineering purposes, with the certainty that consistent results can be produced both by image analysis and by using the available particle analyzer in Parma.

One possibility would be to write the paper from a sedimentological point of view and discuss and compare a series of analyzed sands using the proposed Dw formula, maybe in comparison with other measures such as modes or stripstar results. To include the mineralogical-petrographical analysis of samples would then make sense (the analysis is completely superfluous in the present paper). The definition of Dw, how it compares to other measures and why it is selected, would then go in the appendix. (Many argue that to take the arithmetic mean instead of the mode is the only way to compare grain size measurements with values reported in the literature). A discussion of the particle analyzer settings may also be useful in this context. But even such a paper would improve if one could include the analysis of a few standard samples (made of commercially available glass beads with know size distributions, for example).

I am sure there are other options for re-designing this paper. I would be very interested to see such a paper and, of course, if necessary, to contribute. A possibility for discussion is at the EGU in Vienna, April 14-19, as I will attend (and give a workshop).

Basel, Jan 7, 2024, Renée Heilbronner