Brookhaven Instruments Corporation White Paper

What is a Discrete Particle Size Distribution?[©]

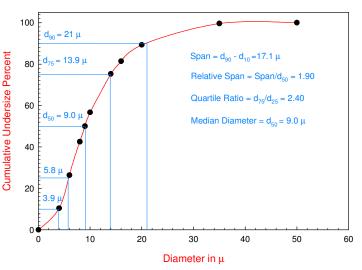
By Bruce B. Weiner Ph.D., May 2011

In the previous entry in this series of papers on particle size and size distribution, the main features of the differential and cumulative size distribution functions were defined and discussed using continuous distributions. Continuous distributions can be measured approximately in fractionation experiments[†] where, for example, data is taken every second as fractionated slices of the distribution pass by a detector yielding size and amount^{*}. Nevertheless, particle sizes are discrete by nature. So let us examine a discrete distribution, one determined by a single particle counter.[‡] Here the "amount" means the number or count or frequency of particles in a size class defined with upper and lower limits.

Size Class in Microns	Count	Percent	Cumulative Percent
0-4	104	10.4	10.4
4-6	160	16.0	26.4
6-8	161	16.1	42.5
8-9	75	7.5	50.0
9-10	67	6.7	56.7
10-14	186	18.6	75.3
14-16	61	6.1	81.4
16-20	79	7.9	89.3
20-35	103	10.3	99.6
35-50	4	0.4	100.0
>50	0	0.0	100.0
Totals	1000	100%	

Cumulative Distribution Tabular Format: There are 1,000 total particles counted (2nd column) and so it is easy to calculate the percent in each class (1st column) simply by moving the decimal point one place to the left (104 becomes 10.4%, 3rd column). And the cumulative percent undersize (4th column) is obtained by adding the current percent in size class to the total above it. Thus, the first one is 10.4%; the second is 10.4% + 16.0% = 26.4%; the third is 16.1% + 26.4% = 42.5%; and so on until one reaches 100%.

Cumulative Undersize Discrete Distribution



Cumulative Distribution Graphical Format: If we plot the cumulative percent vs the upper limit of each size class, we obtain the cumulative undersize distribution. See plot above.

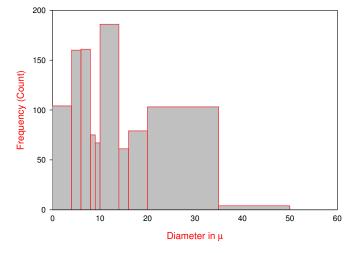
The example here is made up of 10 size classes of unequal size, which has consequences when the frequency distribution is discussed. But first let us discuss the cumulative undersize distribution as it is the more straightforward when there are relatively few size classes.



The percentile diameters were read from the graph; however, in this particular example, they could have been estimated directly from the tabular data with the median diameter, d_{50} , falling exactly at 9 μ .

The black points are the raw data with one added at zero to guide the eye. The red line is a smoothed version of what the continuous cumulative undersize distribution might look like. Obviously, given so few data points, several other smoothed curves could have been drawn. Or, if you assumed you knew the simple functional form of the cumulative undersize distribution, you could have done a nonlinear least squares fit to it. Problem: Most size distributions don't fit simple functional forms. Occasionally some do, like a Lognormal (two parameters), but not many.

If you don't have a simple functional form that you can differentiate, or you have too few data points such as is the case here, then numerical differentiation is extremely suspect. In that case, how do you obtain the equivalent of the differential size distribution in order to determine mean, mode, and measures of width? Answer: Start with a histogram:



Histogram of Frequency vs Particle Size

Histogram of the Frequency Distribution: The plot shows the count (the number) of particles (2^{nd} column) vs size class (1^{st} column) . In statistics this is called the frequency of occurrence in each size class. But it doesn't look much like a size distribution, does it? The reason is simple: The size classes are not all equal and so until we do something to fix that, we can't discern anything analogous to the differential size distribution shown in the preceding paper in this series.

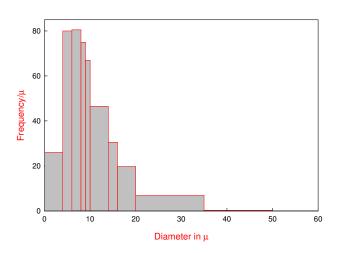
To remedy the situation, divide the count by the size class width. This yields the Frequency/micron (3^{rd} column in table below). This allows us to compare distributions made with different size classes.

Size Class in Microns	Count	Frequency per μ	Fraction per μ
0-4	104	26.0	0.0260
4-6	160	80.0	0.0800
6-8	161	80.5	0.0805
8-9	75	75.0	0.075
9-10	67	67.0	0.0670
10-14	186	46.5	0.0465
14-16	61	30.5	0.0305
16-20	79	19.8	0.0198
20-35	103	6.87	0.0687
35-50	4	0.267	0.0003
>50	0	0	
Total	1000		



Brookhaven Instruments 750 Blue Point Road Holtsville, NY 11742-1832 USA Tel: +1(631)758-3200 Fax: +1(631)758-3255 info@BrookhavenInstruments.com www.BrookhavenInstruments.com **Plot of Frequency/\mu vs. Size:** A plot of the 3rd column vs size class (1st column) begins to look like a size distribution:





You can see a modal diameter somewhere near 6μ . And you can calculate a mean diameter as

follows: $\overline{d_n} = \frac{\sum_{i} N_i \cdot d_i}{\sum_{i} N_i}$, where N_i is the value in

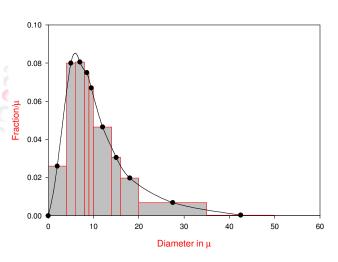
the 2^{nd} column, the frequency (count or number) of particles, and d_i is the midpoint of the class size from the 1^{st} column. Sum over i size classes from 1 to 10, and the result is the number or count mean diameter of 10.8 μ .

You can even estimate the full width at half maximum: Since 80 is approximately the maximum value, 40 is half. Draw a horizontal line at 40. It crosses the unimodal plot at 4 μ and 14 μ . Thus, the FWHM = 10 μ and the HWHM = 5 μ .

Now the area in any bar represents the total amount, in this case number of particles, in the size class. This is analogous to the area under the continuous differential distribution curve between any two diameters. With a frequency distribution, it was the height of the bar that represents the total number in class. Therefore, with the Frequency/ μ plot representing the equivalent of the differential size distribution, we can again determine mean, mode, FWHM and other measures of size distribution width, absolute and relative. However, here is what we can't do: We can't compare this distribution to another one unless the total number of particles counted was equal.

Plot of Fraction/\mu vs Size: In order to compare distributions with different total counts, we must divide each Frequency/ μ by the total number of particles (1,000). This produces the Fraction/ μ , the 4th column. A vertical bar chart of Fraction/ μ vs. size class looks like this:





Its shape is exactly the same as that of the Frequency/ μ ; however, the y-axis is now fraction/ μ . If you had different measurements, you could overlay them in this type of plot to see if they were equal or not.

One more thing can be done here to show how a discrete Fraction/(Size Class Width) plot begins to resemble a continuous differential distribution. Connect the midpoints of each bar using a smooth, continuous curve. This results in something that looks like the differential size distribution. Though there are many such smooth curves that could be drawn.



Brookhaven Instruments 750 Blue Point Road Holtsville, NY 11742-1832 USA Tei: +1(631)758-3200 Fax: +1(631)758-3255 info@BrookhavenInstruments.com www.BrookhavenInstruments.com Which Discrete Distribution Should I Use To Best Present My Data? If there are relatively few size classes and no reason to believe a particular function fits it well, then only use statistics obtained from the cumulative undersize distribution: median, percentiles, span, etc. These numbers will have the least error.

Summary: Like the continuous distribution case, one can construct a cumulative undersize discrete distribution from discrete tabular data and determine median, percentiles, and measures of distribution width. It is more difficult to construct something akin to the continuous differential distribution.

However, to do so, start with the Frequency vs Size Class table and plot. If all the size classes are equal, then divide by the total amount of particles and create a Fraction/(Size Class) plot. If the size classes are not equal, divide each frequency by its own size class width and then divide by the total amount.

If the number of size classes is adequately large, see if a smooth differential-like distribution can be constructed by connecting the midpoints.

† Sedimentation, both gravitational and centrifugal, field-flow fractionation, hydrodynamic chromatography, etc. are examples.

* The amount could be by number, by surface area, by volume, by mass, by intensity of scattered light. The distributions "weighted" by these quantities are all shifted with respect to one another. The topic of weighting is discussed in another entry in this series on particle sizing.

[‡]Single particle counters include electro- and optical-zone counters, image analyzers, and single particle tracking devices.



