HORIBA Scientific

Technical Note

Algorithm Iterations

TN149

UNDERSTANDING 'CALCULATION LEVEL' AND ITERATIVE DECONVOLUTION

Laser diffraction particle size analyzers use advanced mathematical algorithms to convert a measured scattered light intensity distribution into a distribution of particle sizes. Multiple iterations of the data over the algorithm are used to provide final results. The number of iterations has a significant effect on the final calculated size distribution, so an understanding of the process will allow the end user to make the most appropriate selection.

Introduction

Algorithms are mathematical operations that transform the light scatter pattern measured by the analyzer into a particle size distribution. Modern algorithms use iterative deconvolution routines. Deconvolution is the identification of the contributions of individual components contained in the total light intensity (flux) distribution. Iterations are successive calculations of non-linear equations that approach the measured values more closely with each successive calculation.

The number of iterations (described as calculation level or form of distribution in HORIBA software) has an effect on the final size distribution reported. There are several issues to consider when deciding which value to use.

Light Measurement

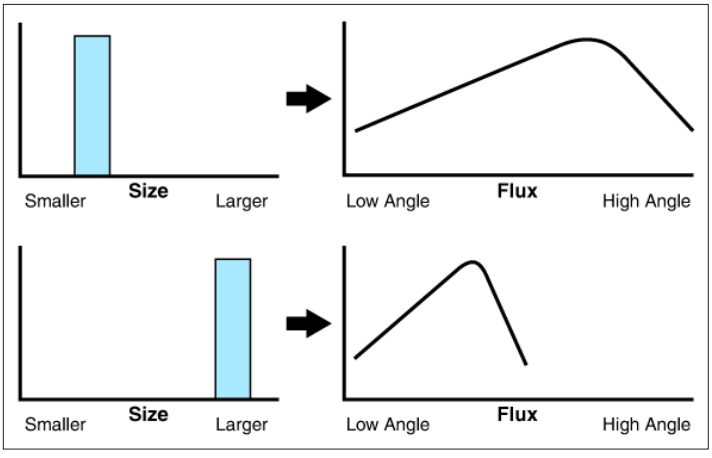

Figure 1. Comparison of size and flux measurement

Light is scattered from the surface of particles at an angle that is dependent on the size of the particle (Figure 1). This light flux is the amount or intensity of scattered light produced at various angles by the presence of particles. Smaller particle sizes scatter at higher angles than larger particles.

For a normal material, there are obviously a range of sizes in the sample. This provides a mix of signals scattered at different angles. The instrument collects this total combined light flux pattern without any way to separate the individual size classes in the sample (Figure 2).

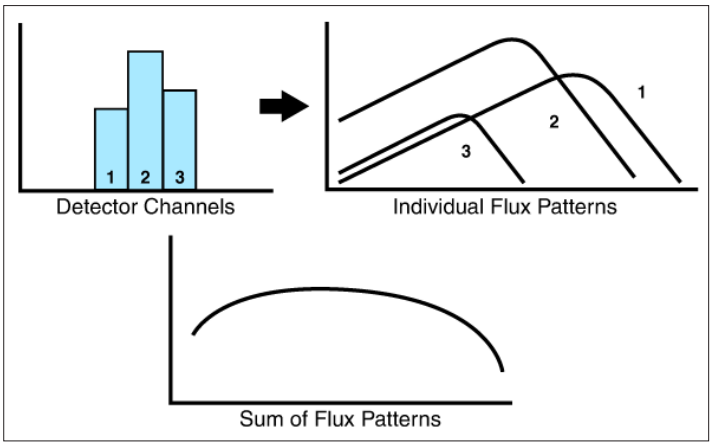

Figure 2. Example of how light flux patterns are collected

Calculation of the size distribution

Modern model-independent calculation algorithms make no assumptions about the distribution; it does not fit the data to a pre-determined distribution form (Gaussian, Rosin-Rammler, etc.).

The Mie Theory, used by all modern laser diffraction analyzers, allows an exact calculation of the light flux pattern from a given size distribution, but does not provide a way to exactly calculate a size distribution from a light flux pattern.

To calculate the size distribution result, the algorithm follows a series of steps to convert from the measured total light intensity distribution (flux) to the particle size distribution. This series of steps is repeated a number of times (iterations). Multiple iterations allow a more accurate result as each iteration reduces the deviation between measured and calculated results (Figure 3).

Each iteration:

1. Makes a calculation (inexact) of the size distribution.
2. Calculates (exactly) what the light flux pattern should be from this size distribution.
3. Compares the calculated light flux against the actual measured light flux.
4. Uses this difference to adjust the size distribution used to make the successive calculations.

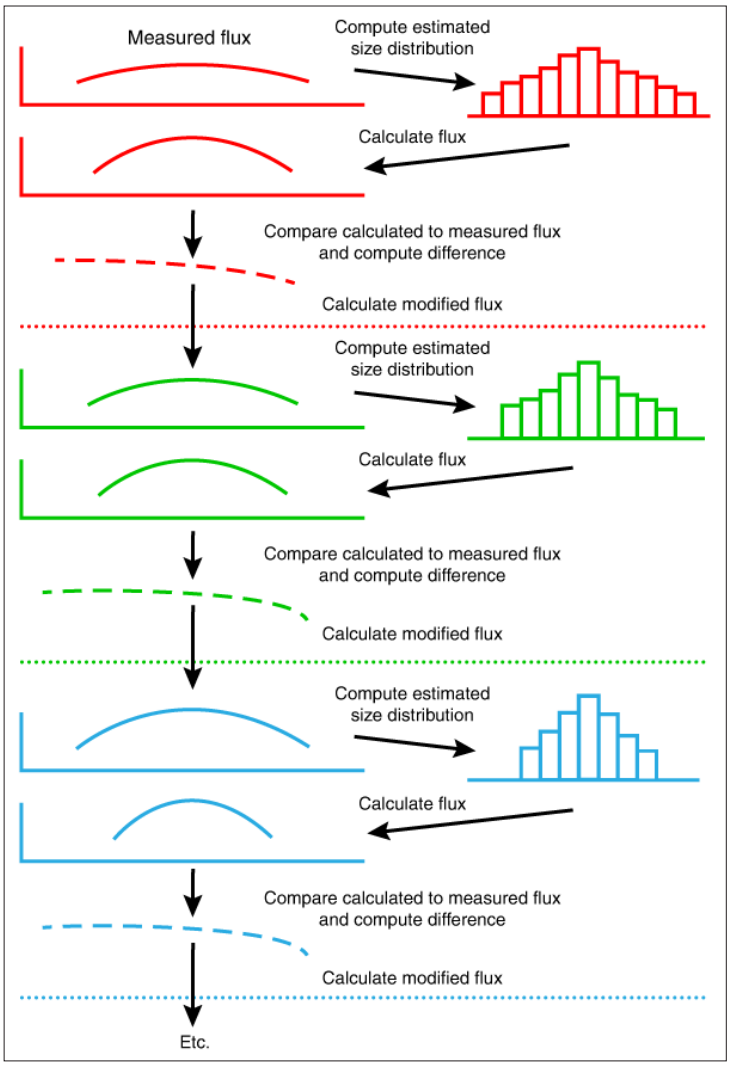

Figure 3. Calculation of size distributions

Limits of Iterations

By iterating the calculation a number of times, the algorithm should theoretically approach a better fit each time. However, the practical limits of the mathematical model mean that iterating without restriction can actually cause the function to diverge, rather than converge to a reasonable result.

To provide a robust solution that is appropriate for the wide range of sample systems a laser diffraction analyzer will measure, a fixed number of iterations are set for the calculation.

For the vast majority of samples, a single default setting provides an accurate measurement of the total distribution, while still providing sufficient resolution to show multiple modes or distributions that do not follow the smooth curve.

All laser diffraction instruments use a similar calculation method. However the user makes this condition selection, the software is following the same basic calculation routine.

Settings for LA-series instruments

Default settings for the different HORIBA laser diffraction models have been made based on the specific algorithm and the response of the optical system. Instead of limiting the user to two or three pre-determined settings, the software also allows the user to manually change to a specific desired number of iterations that would be most appropriate for the sample of interest.

For the LA-960, it was determined that 15 iterations was the most appropriate setting for normal-distribution materials (Standard) and 150 for mono-disperse (Sharp) materials. These values were determined as being appropriate for the vast majority of samples.

Practical Guide for Selecting

Standard mode should be used on all samples unless there is specific knowledge about the distribution and the default setting does not provide expected results.

In general, fewer iterations will yield a broader peak and a greater number of iterations will yield a narrower peak. Caution must be exercised when determining the appropriate number of iterations, as a large number of iterations will resolve distinct peaks in a distribution from what is actually only a small discontinuity.

Increasing the number of iterations increases the resolution of peaks in the results. It should be noted that there are no changes being made to the measurement or the optics; the only change is in the calculations. In a number of cases, such as materials from a classifier or narrow range sieve cuts, a narrow particle size range will be reported, but using Sharp may make this distribution narrower than it truly is.

Example Data

If the material to be tested is manufactured as mono-sized (every particle is exactly the same size), such as certain polymer latex materials, then Sharp mode will help to resolve the distribution in to its correct width. The distribution should be less than one decade (10:1 ratio of smallest particle to largest particle) at the most before we can consider using Sharp mode.

The graph below shows a mono-sized 500 nanometer polystyrene standard in both Standard and Sharp modes. With a narrow distribution material such as this, there is not much difference in the curves, but scanning electron microscopic evidence suggests that Sharp provides the best result.

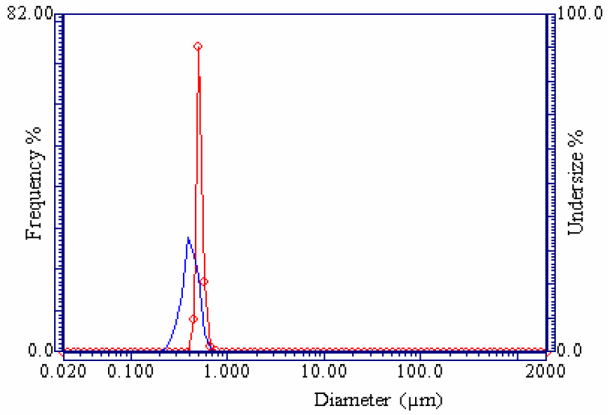

Figure 4. A mono-sized 500 nm polystyrene standard in both Standard and Sharp modes

One other application for Sharp mode is when higher resolution is desired with closely spaced multi-modal distributions. Samples that are known to contain two or three materials might not be resolved in Standard mode, but in the Sharp mode the peaks may be distinctly resolved.

The second graph (Figure 5) illustrates a bi-modal sample calculated in Standard and Sharp modes. A slight “shoulder” in Standard (blue) becomes a distinct peak in Sharp (red). In cases such as this, the user must determine which type of distribution is most accurate.

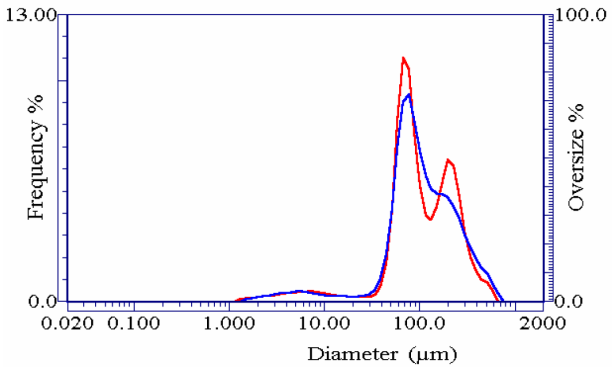

Figure 5. A bi-modal sample calculated in Standard and Sharp modes