Technical Note

Multimodal Report Software

TN170

Particle size distributions are not always single peak, symmetric, or beautiful. In the real world many sample analysis results include two or more distinct populations. Data interpretation can be more difficult for multimodal results. For this reason advanced reporting capabilities are built into the LA-960V2 software as described in this document.

Introduction

When the laser diffraction technique was first introduced the result calculations were limited to constrained calculation models such as log normal or Rosin-Rammler. As computing power increased and algorithms improved result calculations became unconstrained and results were presented in their more true (but messy) form. While data interpretation is now sometimes more challenging, the good news is that more information is available to describe the state of the sample.

Multimodal Report

The LA-960V2 software experiences constant improvement in true Japanese *kaizen* style driven by customer comments and requests. One customer several years ago requested the ability to access improved statistics for their multimodal sample results. This request resulted in the Multimodal Report feature now present in the LA-960V2 software. This feature allows customers to better quantify many details buried in results containing more than one population. Information now available for two or three separate modes includes:

- D10
- D50
- D90
- Mode
- Standard deviation
- Span
- Area ratio
- Frequency distribution for each
- Cumulative on % for each
- % on cumulative for each
- Sum of squares residual

Examples

1. Aggregated pigment

A customer was developing a new method for a pigment that was aggregated in the state as arrived in the lab. Ultrasound was used to disperse the aggregates to the single particle state. When asked to define the degree of aggregation prior to use of ultrasound, the customer presented the multimodal report results that show the statistics for the peak of aggregates. Figure 1 shows the results for the aggregated (blue) and better dispersed (red) samples.

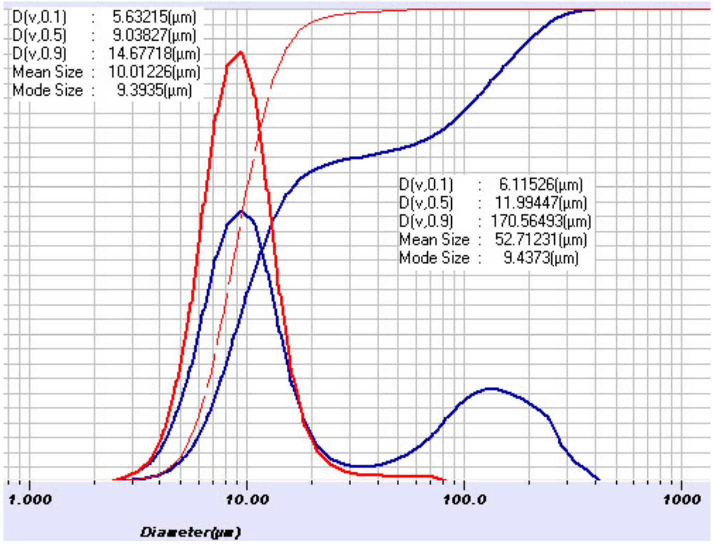

Figure 1: Dispersed (red) and non-dispersed (blue) pigment results.

The multimodal report for the non-dispersed result is shown in Figure 2. From this report, the customer defined the degree of aggregation as 32%, the percent of the total population existing as aggregates.

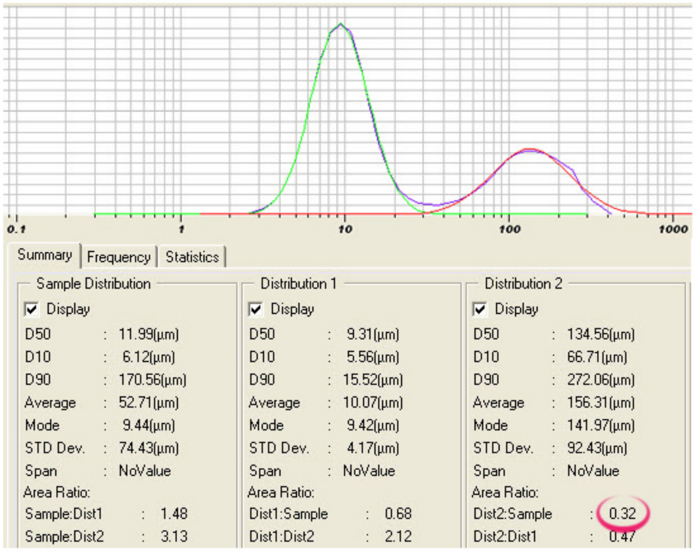

Figure 2: Multimodal report for the non-dispersed pigment

2. Good vs. bad product batches

A customer doing research in the field of PLA nano-particles for drug delivery uses the LA-960V2 to monitor batch quality. The vast majority of the time all particles are smaller than 500 nm, but occasionally, when things go wrong, larger particles (as large as 100 µm) appear. The LA-960V2 is uniquely capable of providing sensitive results across such wide dynamic range. Figure 3 shows a good (red) vs. bad (blue) batch of particles.

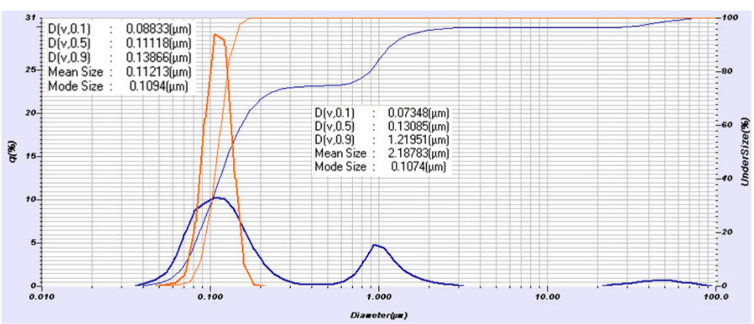

Figure 3: Good vs. bad batch of nanoparticles

The scientists could easily visualize the good vs. bad batch, but the quality control group preferred to quantify the differences numerically. The LA-960V2 multimodal report provided the solution as seen in Figure 4. The proportion of particles in each peak are easily identified and reported, providing clear statistical information to be used for quality control and studies.

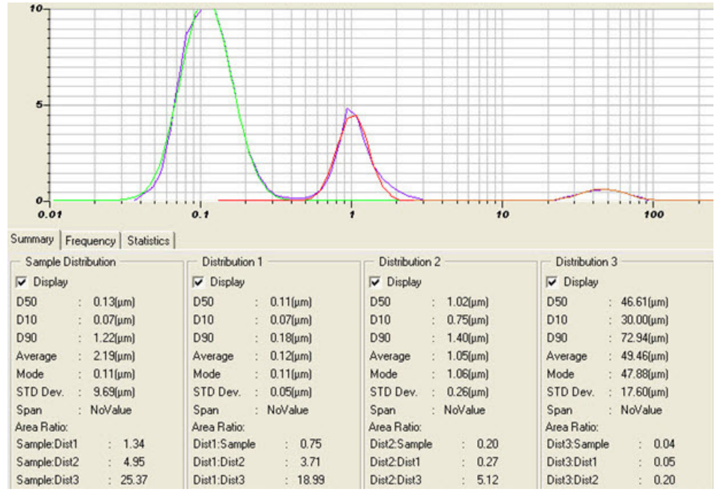

Figure 4: Multimodal report for bad batch of nanoparticles

Conclusions

The LA-960V2 multimodal report provides detailed statistical information for results containing two or three populations. This feature includes a full deconvolution of "mixed" peaks (i.e. no baseline resolution in-between). The deconvolution method is far superior to simply treating each peak as two halves of a whole, cut down the middle. This information can be used in many ways including quality control and degree of aggregation information. The results available are statistically comprehensive, but easily interpreted.