SIZE SURE ON THE MASTERSIZER 3000+: ENHANCING CONFIDENCE IN ROUTINE MEASUREMENTS AND STREAMLINING METHOD DEVELOPMENT

How can you prevent unwanted contaminants from slowing down progress during the measurement of size distributions using laser diffraction?

The answer is to use Size Sure, a software feature available on the Mastersizer 3000+ that reliably differentiates between steady-state and transient signals. With Size Sure, you'll understand your sample better, improve confidence for routine measurements, and get your method development right first time.

The challenge of real-world samples

In an ideal world, dispersions of particles for size analysis by laser diffraction would be completely clean, and the analytical process would run without a hitch to generate particle size distributions (PSDs) that accurately reflect the true sample.

But analyses in real life are rarely that simple. For example, many of us will know the frustration of finding bubbles or aggregates in the dispersion liquid halfway through sample preparation or analysis. Not only that, but if the particles you're studying have a tendency to adhere to the dispersion accessory walls or other surfaces, it's all too easy for one sample to contaminate the next, even when you're following cleaning protocols carefully.

The result of these unwanted particles – so-called 'transients' – is to modify the diffraction pattern generated at that point in time, generating PSDs that can be misleading. When making routine measurements, this can reduce reproducibility and raise unnecessary doubts over the quality of the source material. And if it happens at the early stage of method development, it can send your whole optimization process off-course, wasting time and generally making life difficult.

Does this sound familiar? If so, then help is at hand, thanks to the Size Sure feature now available with the Mastersizer 3000+ from Malvern Panalytical.

About the Mastersizer 3000+

Since its launch in 2012, the Mastersizer 3000 laser diffraction system has gained a well-deserved reputation as a high-performing, versatile and compact instrument for obtaining particle size distributions.

With applications including assessing powder flowability and packing, understanding drug dissolution rates, monitoring food emulsion stability, and ensuring optical performance of paints, Mastersizer 3000 has become a valuable tool throughout R&D and manufacturing. This success is down to both the hardware and the software: over the years, as well as numerous features and accessories, we've released two software modules that benefit all Malvern instruments – Smart Manager for optimizing uptime and usage, and OmniTrust for ensuring regulatory compliance and data integrity.

The Mastersizer 3000+, launched in March 2024, continues this tradition, with three added software features to enhance your particle-sizing capabilities and inform your critical decision-making:

- Size Sure for improved confidence in routine measurements and method development
- Data Quality Guidance for helping you to make independent decisions on real-world samples
- SOP Architect for standardized, streamlined method development.

Add to these features the instrument's flexibility and ease of use, and the Mastersizer 3000+ truly becomes the top choice for particle sizing.

Click on the links above for more information on each of these features, or contact us to enquire about the Mastersizer 3000+.

Size Sure on the Mastersizer 3000+

Unique to Malvern Panalytical, the Size Sure measurement mode is only available on the Mastersizer 3000+, and uses an efficient patent-pending machine-learning approach (known as Adaptive Diffraction) to classify data into two states, reported separately:

- **Steady-state data** describes the particles that are observed most of the time
- **Transient-state data** describes any events – from particles or otherwise – that are only observed occasionally, typically less than 10% of the time.

The measurement mode is enabled by selecting the 'Size Sure' option in the software, and this then generates two PSDs in the final report (Figure 1). The result is that the steady-state data is inherently more representative of the true sample, giving you greater confidence in your results. And at the same time, the fact that the transient-state data is reported separately enables you to understand the data better, and take action to minimize these interferences in future analyses.

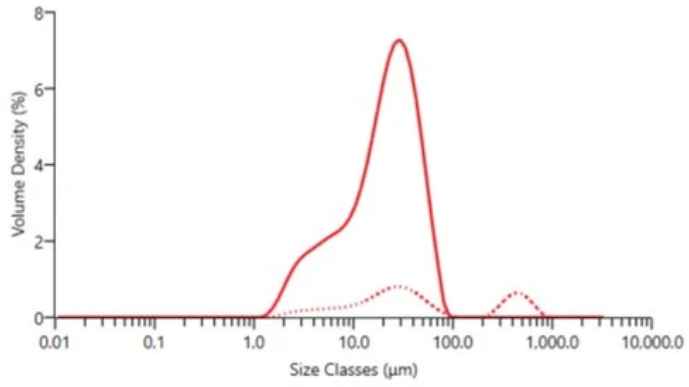

Figure 1: Particle size distribution for an ibuprofen suspension measured in the presence of interfering transient scattering events using Size Sure, showing the steady-state (solid line) and transient-state (dotted line).

Crucially, Size Sure is not behaving as a data filter – all it's doing is generating two PSDs where previously you would have had to make do with just one. And because these PSDs are derived by simply 'splitting' the original data, you can sum them using the 'Extract Classic Result' function to generate the classic PSD. By the way, although Size Sure can help screen out the effect of transients, we wouldn't recommend using it as an excuse for being less rigorous about sample cleanliness (sorry to break the bad news).

How does Adaptive Diffraction work?

Within the Adaptive Diffraction algorithm, the raw diffraction data is combined into segments on a millisecond timescale. These segments are classified as either 'steady-state' or 'transient-state'. The segments within each class are then averaged over the whole length of the measurement, before application of Mie theory or Fraunhofer theory to turn them into a PSD. The Adaptive Diffraction classification uses machine-learning algorithms to adapt the processing parameters during the course of the measurement. These algorithms are not memory-intensive, meaning that they will run quickly and reliably on the same computer used for instrument control. And because we've validated the results on 1 TB of diffraction data (which took a while, take our word for it!), you can have confidence in the results.

Key applications of Size Sure

Size Sure has benefits for all sample types. It's particularly valuable in environments where contamination of dispersant is often observed, and where maintaining a perfectly clean lab is challenging – for example, in ore extraction, cement production, or large-scale polymer processing. It's also useful where you're encountering cross-contamination with previous samples, for example when particles are susceptible to adhering to the cell walls.

To exemplify how Size Sure copes with these situations, Figure 2 shows its use to differentiate between latex particles and a very small number of larger glass beads representing a contaminant.

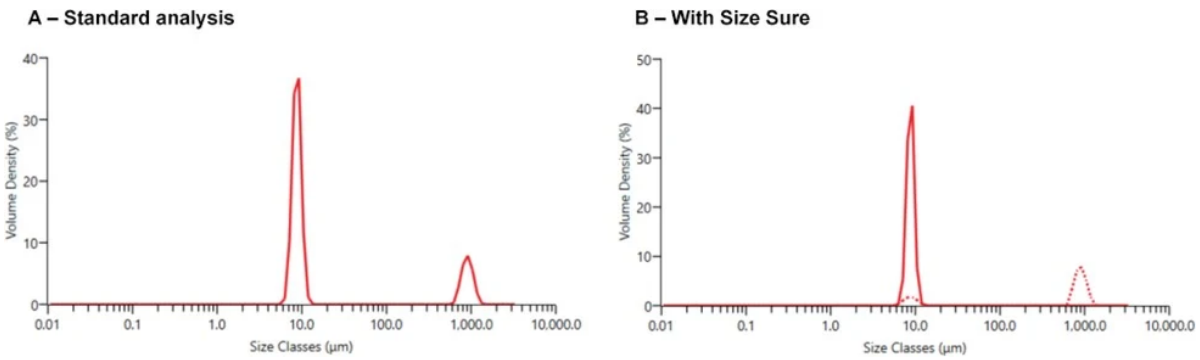

Figure 2: Particle size distributions obtained for an 8.9 µm latex sample spiked with three 1 mm glass beads, representing a coarse particle contaminant: (A) Standard analysis, showing an apparently bimodal distribution as a result of the presence of the contaminant; (B) Analysis using Size Sure, showing the separation of the contaminant as the transient state (dotted line), enhancing confidence in the distribution of the latex particles as the steady state (solid line). Note: In plot B, the reason for a small portion of the 8.9 µm band being identified as 'transient' is that any data segment generated from a part of the sample containing a transient particle will also contain regular particles, making it impossible to completely separate out the two signals.

Another situation where Size Sure is useful is when bubbles form within your sample dispersion, which is especially common when you're using surfactants to aid dispersion. Figure 3 shows how Size Sure can pick up on such artefacts, using sparkling water as the dispersant to mimic bubble formation in a sample of glass beads.

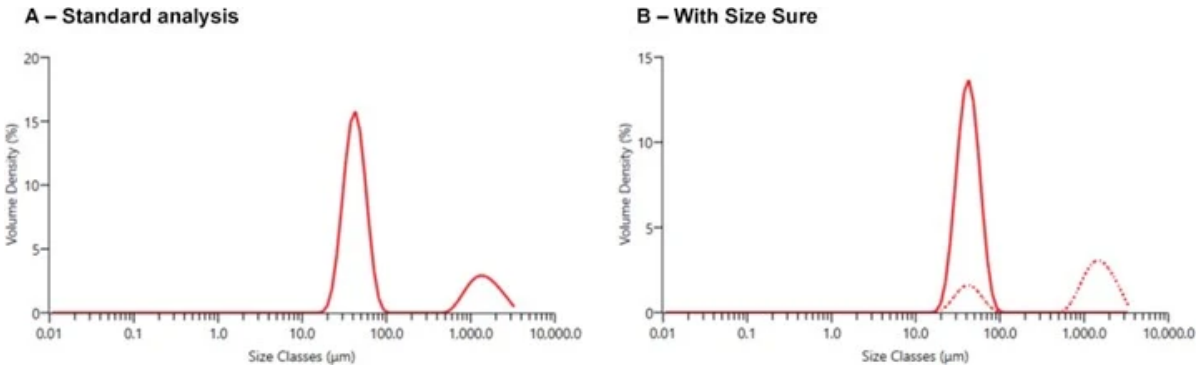

Figure 3: Particle size distributions obtained for a sample of glass beads with a Dv50 of 42 µm, using sparkling water as the dispersant to mimic a source of bubbles: (A) Standard analysis, showing the main mode from the glass beads on the left, but with an additional peak to the right caused by the presence of bubbles in the measurement; (B) Analysis using Size Sure, showing separation of the bubbles into the transient state (dotted line), enhancing confidence in measurement of the glass beads as the steady state (solid line).

Whatever the cause of transient signals in your analysis, Size Sure has greatest value in the following situations:

- During routine analysis, when the aim is to maximize the reproducibility of your results, and not have your confidence in the data unnecessarily impacted by a rogue coarse particle or bubble.

- At the beginning of method development (or during early-stage screening studies), where it's essential to know whether an unexpected mode in the PSD is part of the true particle distribution, or whether it simply reflects the presence of a rogue coarse particle or bubble.

Depending on your priorities, once Size Sure has identified a transient, at that point you might want to look at it in more detail (for example, using the Hydro Insight dynamic imaging accessory for the Mastersizer) as shown in Figure 4.

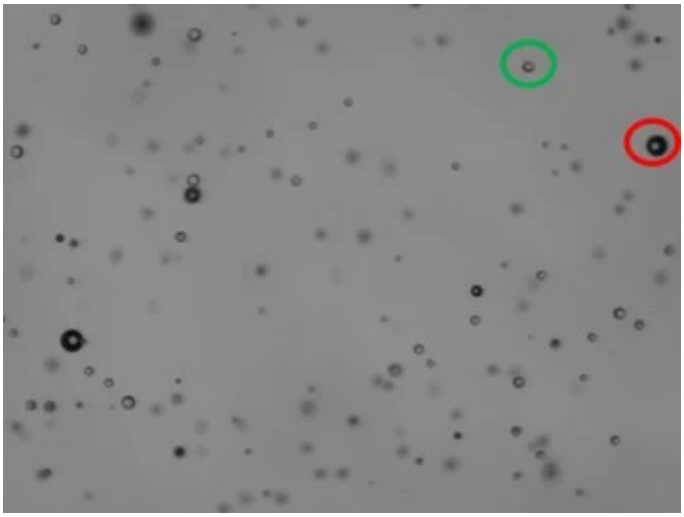

Figure 4: Example Hydro Insight image showing glass beads (example circled in green) and bubbles (example circled in red).

Or if you're doing method development, you might simply want to press ahead with further work (for example, using the SOP Architect module on Mastersizer 3000+), safe in the knowledge that your initial conclusions are on a firm footing.

Size Sure can also work hand-in-hand with the Data Quality Guidance software module available on the Mastersizer 3000+. This detects a range of common data quality issues, and gives you prompt feedback on them, which is great if you're building up your experience with laser diffraction.

Conclusion

By separately reporting on data acquired during the passage of 'transient' particles such as dust, bubbles and aggregates, Size Sure:

- Gives you greater confidence in your steady-state size distributions during routine analysis

- Enables you to streamline early-stage method development

- Help you understand the nature of any transients

- Avoids having tight analytical schedules derailed by contaminants.

Interested in using the power of Size Sure to help your analyses? Talk to us today about the Mastersizer 3000+.

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