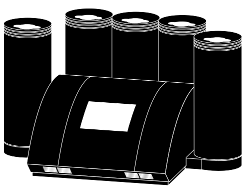
Application Note

Multiscan Stability Index (MSI)

-One-click stability evaluation-

The MultiScan MS 20 (Fig. 1) from Dataphysics Instruments serves as an invaluable analytical instrument, offering comprehensive insight into the stability of any given dispersion formulation. The stability data is obtained by observing the evolving intensity of backscattered and/or transmitted light over a specified time frame. It can be difficult to conduct an objective analysis of the data in the absence of input from a qualified expert in cases where simultaneous destabilisation phenomena occur, such as sedimentation and aggregation. In response to this challenge, Dataphysics Instruments has developed a straightforward yet robust criterion, the Multiscan Stability Index (MSI), which enables the rapid comparison and characterisation of formulation stability. This application note describes the calculation of the MSI and provides illustrative examples of its use.

Measurement device
MultiScan dispersion stability analysis system



Measurement method
Optical dispersion stability analysis

Measured quantities
Transmission intensity
Backscattering intensity

Environmental conditions
25 °C

Samples
Dispersion formulations

Industries
All dispersion formulations

MultiScan Technique

The MultiScan MS 20 technology is based on the static multiple light scattering (SMLS) principle (Fig. 2).[1] To conduct the measurement, the liquid dispersion is poured into a sample vial, which is then placed in one of the measuring chambers of the MultiScan MS 20. The MS 20 apparatus comprises a light source, a detector positioned opposite the light source for measuring the transmitted light, and a second light source, oriented at a 45-degree angle from the detector, for measuring the backscattered light. During each measurement, the light sources and detector move up and down along the sample vial, the signals transmission (Tr) and backscattering (BS) are obtained by repeated measurement at the full sample height h over a period of time t. This is achieved by a scanning process from position z = 0 to z = h, with a step size of Δh. The resulting signals are Tr (t, z) and BS (t, z), which are functions of time t and height z. The composition of these scans enables the detection of physical instabilities in the dispersion process, including aggregation, sedimentation and creaming amongst others.

MSI Definition

It is of great importance to classify and compare the stability of numerous formulations in a quantitative manner. A comparison of the stability of formulations based solely on the raw Tr or BS signals may necessitate the utilisation of sophisticated computational techniques. This is why the MSI has been introduced as a means of overcoming the aforementioned limitations. The MSI can be employed to achieve this with a straightforward method, resulting in a single number that describes the global sample stability. The MSI is a numerical value calculated at a specific point in time t by aggregating all temporal and spatial variations of the Tr and BS signals.

Fig. 1: DataPhysics Instruments stability analysis system MultiScan MS 20 with six independent ScanTowers

$$MSI\ (t) = \sum_{t_{j=1}}^{t_{max}} \frac{\sum_{z_i=z_{min}}^{z_{max}} |TrBS(tj,zi) - TrBS(tj_{-1},zi)|}{z_N}$$

t_{max} represents the measurement point corresponding to the time t at which the MSI is calculated. z_{min} and z_{max} denote the lower and upper selected height limits, respectively. z_N is defined as $(z_{max} - z_{min})/\Delta h$, the number of height positions in the selected zone of the scan. TrBS represents the considered signal (BS if Tr < 0.1%, Tr otherwise).

It can be seen that the sample is stable when the MSI tends towards zero and more unstable with growing MSI.

Additionally, an MSI scale, which correlates with the visual variation of the sample, has been provided. Fig. 3 shows the bars in the graph are coloured in accordance with the scale presented below the graph, which utilises a colour code and a grade to indicate the level of destabilisation. This

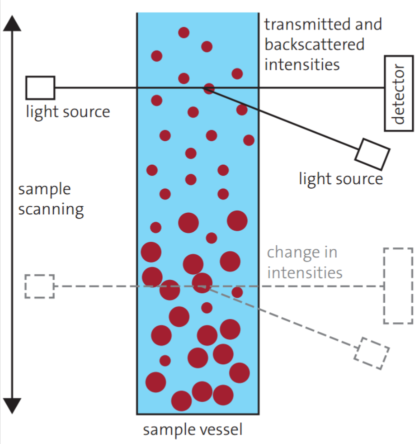


Fig. 2: MultiScan measuring principle

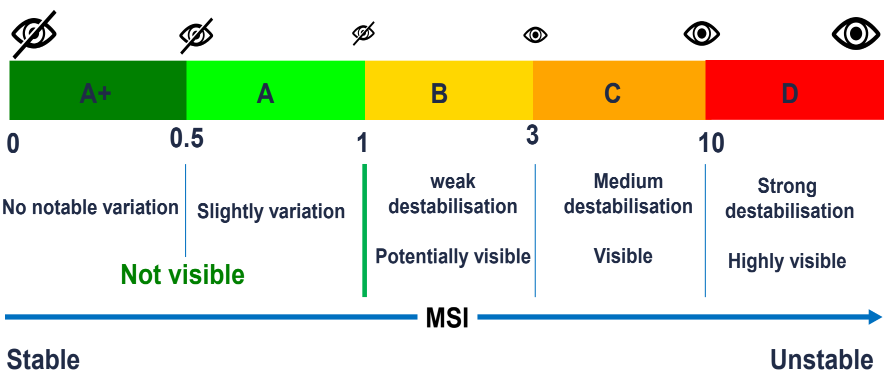


Fig. 3: The MSI scale employs a colour coding system, with each bar on the graph displaying a specific colour and grade according to the level of destabilisation.

scale is based on an empirical analysis of a database comprising hundreds of measurements.

Experiment

20 ml of each formulation were homogenised using a shaker and poured in a transparent glass vial to be measured at T = 25 °C every 6 minutes for 28 hours. The measured zone was between 0 mm (bottom of the glass) and 57 mm (top of the glass vial).

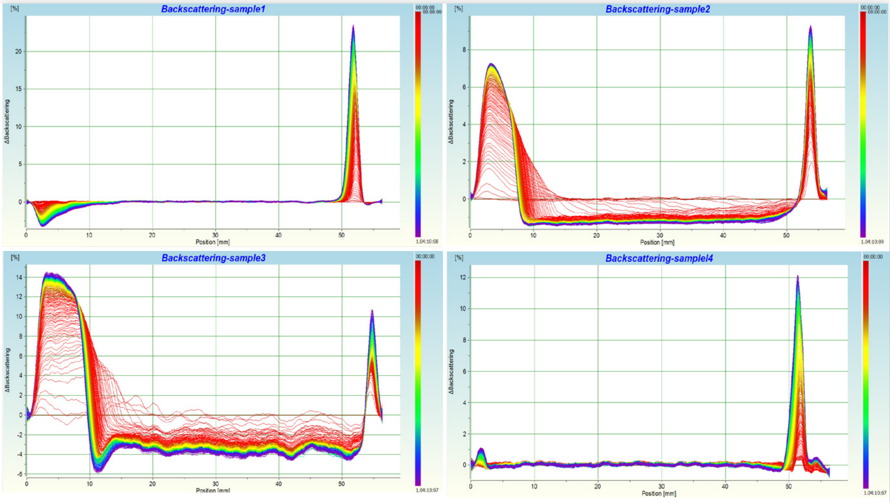


Fig. 4: The backscattering intensities of four samples in relative scale against the position

Results & Discussion

Fig. 4 shows the backscattering intensities in relative scale against the position for the four samples. The color-coding of the curves indicates the time at which they were recorded, from red (first measurement, t = 0 s) to purple (last measurement, t = 28 h). Every curve represents an individual measurement.

The backscattering diagrams illustrate a time-dependent and position-dependent alteration of the signal, which is induced by changes in particle size or particle migration. The backscattering intensities of Sample 1 demonstrate an increase at the top layer and a decrease at the bottom layer, indicative of a creaming process. The backscattering intensities of both Sample 2 and Sample 3 display an increase at the bottom layer and top layer, while a decrease is observed at the middle layer. This indicates that a creaming process is occurring at the top layer, while a sedimentation process is taking place at the bottom layer. The middle layer of Samples 3 and 4 undergo clarification as a result of particle migration from the middle layer to the top and bottom layers. A slight decrease in the backscattering of Sample 4 at the bottom layer indicates the occurrence of a relatively minor sedimentation process. Furthermore, the backscattering intensities of Sample 4 demonstrate an increase at the top layer, which suggests that a creaming process is occurring.

As outlined in the MSI definition, MSI global represents a numerical value calculated at a specific temporal point, by aggregating all temporal and spatial variations across the entire sample height. The method is capable of classifying and comparing the stability of a variety of formulations in a quantitative manner, without regard to the underlying destabilisation mechanisms. Fig. 5 (left) illustrates that the MSI global of the samples undergoes a temporal change. The MSI value of Sample 3 is the highest among the samples during the measurement period, indicating that it is the most unstable formulation. The MSI values of Samples 1 and 4 are significantly lower than that of other samples, indicating that Samples 1 and 4 have the highest stability within the specified measurement period.

In addition, the MSI histogram based on the MSI scale allows the assessment of the degree of destabilisation at a given time. For example, Fig. 5 (right) shows the MSI values for the four samples at the measurement time of 24 hours as a histogram.

To more clearly understand the destabilisation occurring in a given area, the MSI zone function was developed. Fig. 6 (upper) shows the variation of MSI in the bottom, middle and top layers of the samples over time. Sample 3

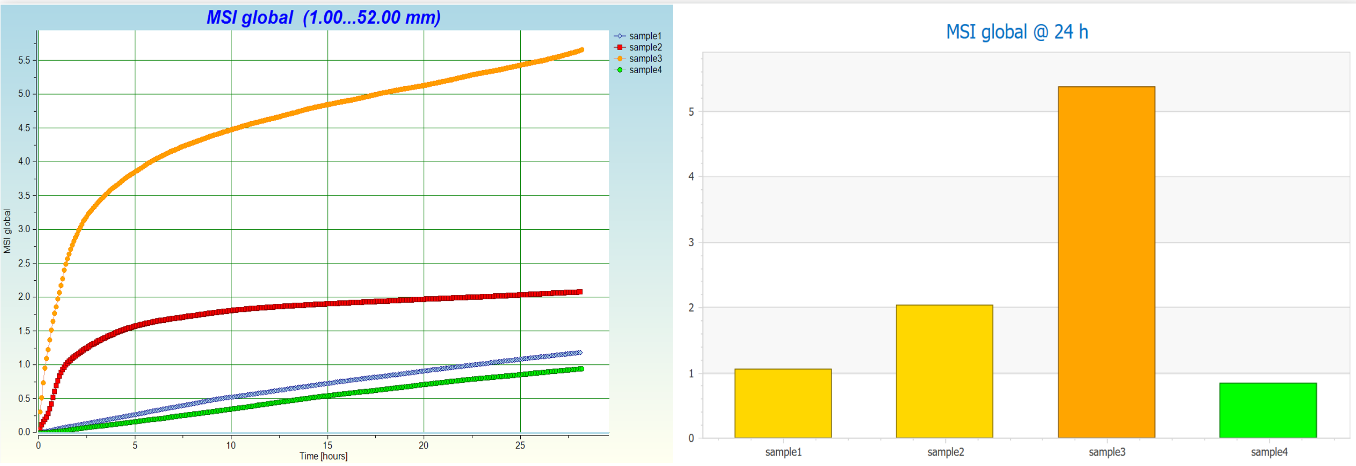


Fig. 5: Left: The change of the global MSI over time; Right: The MSI values for the four samples after the measurement time of 24 hours in histogram form

shows pronounced instability in the lower layer and significant destabilisation in the middle and upper layers. Both Samples 1 and 4 show a relatively stable behaviour at the bottom and middle layers, while their top layer shows a relatively unstable behaviour. Fig. 6 (lower) presents the MSI zone values after 24 hours measurement time in the histogram form. According to the MSI scale, there is no discernible change in the middle layers of Sample 1 but a change can be observed in its bottom and top layer. There is a visible change in the bottom layer of Sample 2, and no visible change occurs in the top layers. The bottom layer of Sample 3 shows a strongly visible change, while the middle and top layers show noticeable changes. In Sample 4 there is no visible change in the bottom and middle layers, but the top layer is likely to show a change.

It is important to note that the MSI methodology accounts for all potential destabilising factors present within a sample, including the presence of bubbles and syneresis, as well as any size variation.

Summary

The MSI is a straightforward and reliable parameter that enables direct and quantitative assessment of the stability of any formulation. It is a time- and position-independent value of the global or zone-specific signal under consideration. It provides a simplified approach to objectively compare and rank the stability of formulations, thus facilitating the sample characterisation. The MSI can be employed as a stability criterion and classification number.

Reference

[1] https://www.dataphysics-instruments.com/products/ms/

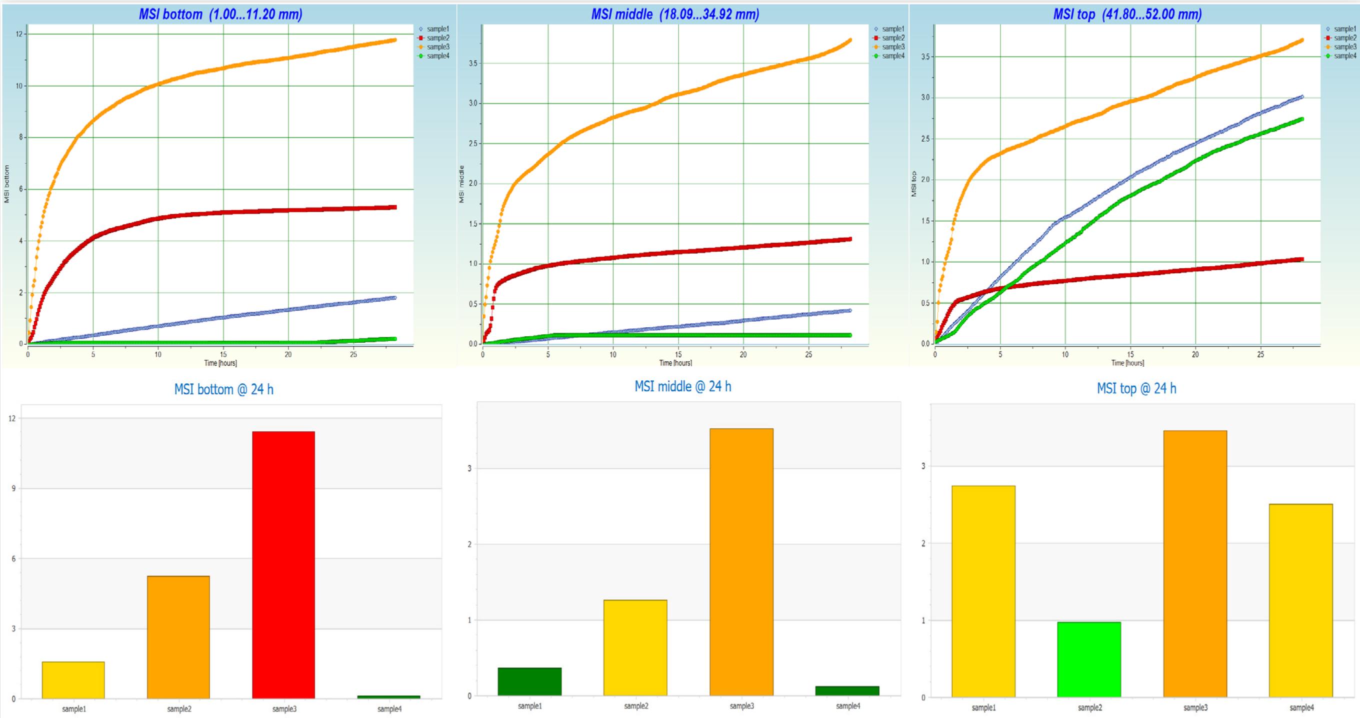


Fig. 6: Upper: The variation of MSI in the bottom, middle and top layers of the samples over time; Lower: The MSI zone values after 24 hours measurement time in histogram form

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