Brookhaven Instruments Corporation

White Papers • Application Notes • Theory Guides

Part 3: The New Customizable Correlator Layout - Channels

Contents

Correlator

The correlator is a crucial part in dynamic light scattering (DLS) instrumentation and helps facilitate accurate measurement of particle sizes. Brookhaven Instruments has introduced an upgraded correlator to enhance DLS measurements.

The autocorrelation function (ACF) is a mathematical algorithm employed to measure the resemblance between a signal and a version of itself shifted in time. In DLS, scattered laser light intensity is transformed into an ACF to measure particle size distribution. This method analyzes rapid intensity fluctuations resulting from the Brownian motion of dispersed particles. The ACF, the raw data in DLS, is utilized to calculate effective diameter and polydispersity index (PDI) through Cumulants analysis.

Additional information regarding a sample can be obtained using the ACF, including a size distribution curve.

A New Customizable Correlator Layout

A unique feature found in Particle Solutions v4 that is not found in other DLS instrumentation is the ability to customize the correlator layout for samples measured using forward scatter, side scatter, or backscatter detection angles. The ability to modify the number of channels, as well as the first and last delay, is especially useful with samples that have a very slow decay rate due to very low mobility whether due to size of the particle or viscosity of the diluent used in sample preparation.

In the following study, we examine the Channels feature of the advanced correlator layout of Particle Solutions v4.

What are Channels?

Modifying the number of channels in a correlator layout allows for changes in resolution. Reduced resolution may be desirable if an ACF is too noisy, due to either weak scattering or short measurement duration. Removing channels can minimize the risk of overfitting noisy data. Particle Solutions 4 now contains a section in the SOP called Correlator Layout (Advanced). Two subsections fall under this category, the first is the Requested Layout **(Figure 1)** and the second is the Verified Layout **(Figure 2)**.

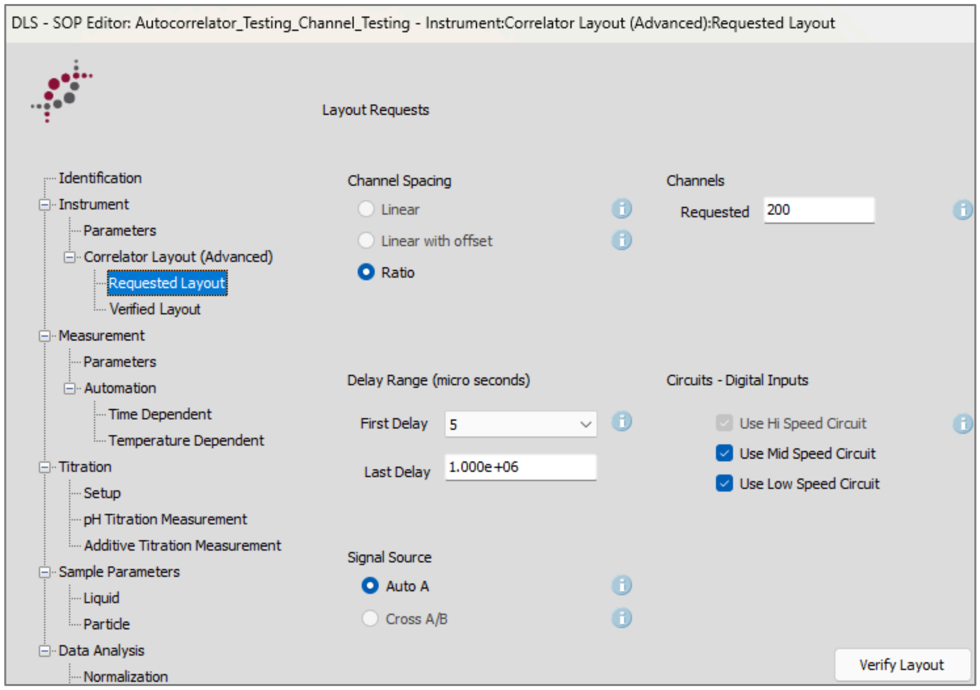

Figure 1: Particle Solutions SOP window containing the Correlator Layout (Advanced) feature. In the Requested Layout section, users can input the requested number of channels.

Requested Layout allows the user to request a specific number of channels, essentially the number of points on the autocorrelation function, in between the first and last delay time. The correlator configuration tool will attempt to configure the high-, mid- and low speed channels to provide the requested number of channels.

The Verified Layout feature will display the actual number of achievable channels for a given correlator layout.

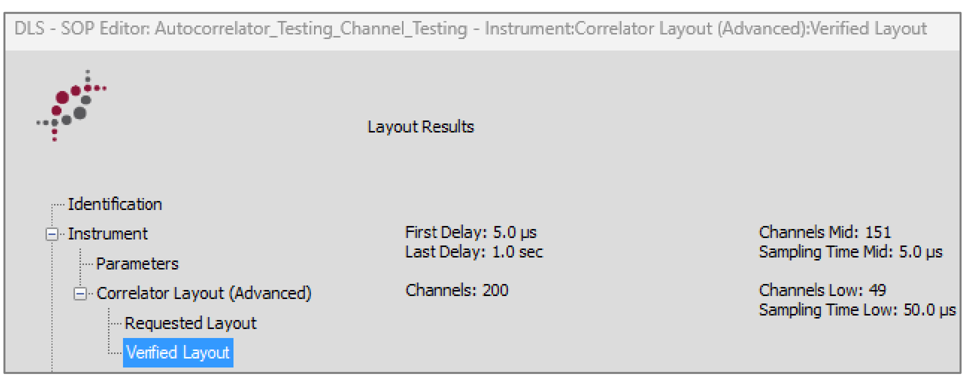

Figure 2: Particle Solutions SOP window containing the Correlator Layout (Advanced) feature. In the Verified Layout section, users can confirm their requested layout and the maximum number of channels that can be set.

Effect of Channel Selection on the Autocorrelation Function

Experimental Methods

The impact of changing the number of channels, using the advanced correlator layout feature of Particle Solutions, on the resolution of particles of various sizes in a sample, was studied using a single sample containing both 88 nm and 600 nm Polystyrene Latex (PSL) Standards diluted in 10 mM KNO_3.

The 600 nm PSL particles were diluted to obtain the same count rate as that of 1 drop of 88 nm PSL in 20 mL of 10 mM KNO_3.

The first and last delays were kept constant at the default values of 5 µs and $1.0x10^6$ µs, respectively, as seen in **Figure 1.** The samples were measured using the following channels: 20, 50, 150, 200 (default), 250, 316 (highest possible with default first and last delays). Since two particles are being measured at the same time, the diameter of each individual peak was evaluated rather than the effective diameter, which is the average of the two peaks. Additionally, the graphs were used to obtain a visual of what Particle Solutions is measuring from the sample at each requested channel.

Note: The following measurements were performed using the 90° scattering angle, which has a default first delay of 5 µs.

Results

Default - 200 Channels

Table 1 displays the results for six replicates measured using 200 channels, and **Figure 3** displays the multimodal size distribution (MSD) of the sample. To learn more about Data analysis and distribution weighting, see our FAQ. The default MSD setting represents intensity-weighted results for each population size in a sample. From the intensity weighted results, it is apparent that there are two peaks. The mean diameter for peak 1 is 85.94 nm ± 2.05 nm, and the mean diameter for peak 2 is 669.66 nm ± 333.06 nm. The percent relative standard deviation (%RSD) was calculated for each peak and the %RSD for peak 1 is 2.4% while that of peak 2 is 49.7%.

The changes in %RSD are seen in the graphs for each peak. With Peak 1, the six replicates fall into a single overlapping peak, which resulted in a lower standard error. For Peak two, the six replicates do not overlap each other and resulted in a higher standard error.

With the new advanced correlator layout, the number of channels can be modified to optimize the measurement. By optimizing the channels, it is possible to determine if the standard error can be reduced for one or both peaks. The following results show the influence of the Channel numbers below and above the default of 200 and the impact of the standard error for both peaks.

	DLS							
Sample ID	Peak 1 Diam. by Int (nm)	Peak 2 Diam. by Int (nm)	Polydispersity	Baseline Index	Count Rate (kcps)	Data Retained (%)	Diffusion Coeff. (cm^2/s)	Rel. Variance By Surface
Mean:	85.94	669.66	0.215	6.9	473.9	98.59	4.297e-08	0.96
Std Err:	0.84	135.97	0.006	1.1	2.1	0.63	4.567e-10	0.19
Std Dev:	2.05	333.06	0.015	2.8	5.2	1.55	1.119e-09	0.47

Table 1: *Results of sample containing 88 nm and 600 nm PSL particles measured with 200 channels.*

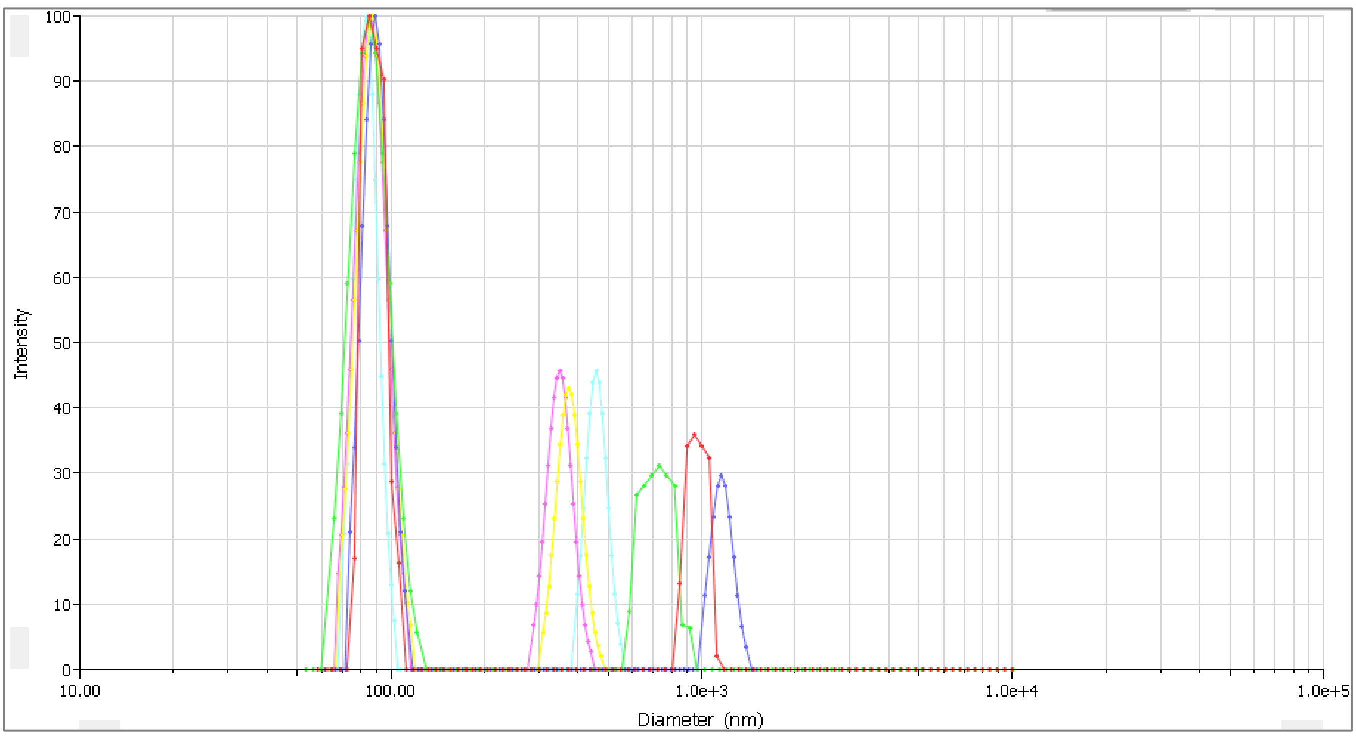

Figure 3: *MSD of sample containing 88 nm and 600 nm PSL particles measured with 200 channels.*

20, 50, 150, 200, 250, and 316 Channels

After measuring the sample containing both the 88 nm and 600 nm PSL particles using the default setting of 200, it was observed that the 200 channels configuration was not optimal. The sample was measured with other channels settings including: 20, 50, 150, 250, 316 to determine if the number of channels affects the distinguishability between multiple peaks and repeatability of each peak. **Table 1** is a summary of data collected from Particle Solutions v4 at the various channels, including peak 1 and 2 mean diameters, standard deviations, and %RSD values. Six replicates were taken at each channels setting.

Peak 1 88 nm PSL Results						
Number of Channels	**20**	**50**	**150**	**200**	**250**	**316**
Mean Peak 1 Diam. (88 nm PSL)	67.93	95.69	89.29	85.94	76.69	52.01
Standard Deviation	33.46	10.78	4.59	2.05	29.46	14.04
%RSD	49.3%	11.3%	5.1%	**2.4%**	38.4%	27.0%
Peak 2 600 nm PSL Results						
Number of Channels	**20**	**50**	**150**	**200**	**250**	**316**
Mean Peak 2 Diam. (600 nm PSL)	324.39	659.81	537.77	669.66	453.97	162.82
Standard Deviation	244.51	164.91	103.60	333.06	268.93	47.58
%RSD	75.4%	25.0%	**19.3%**	49.7%	59.2%	29.2%

Table 2: *Mean diameters, standard deviations, and %RSD for peak 1 and 2 were obtained from testing a sample containing 88 nm and 600 nm PSL particles at various channels settings. Six replicates were measured at each number of channels setting.*

Results indicate that 200 channels resulted in the lowest %RSD for peak 1 while 150 channels resulted in the lowest %RSD for peak 2.

Graphical representations of the mean diameters for peak 1 and 2 and their respective standard deviations, found in **Table 2,** can be seen in **Figures 4 and 5**.

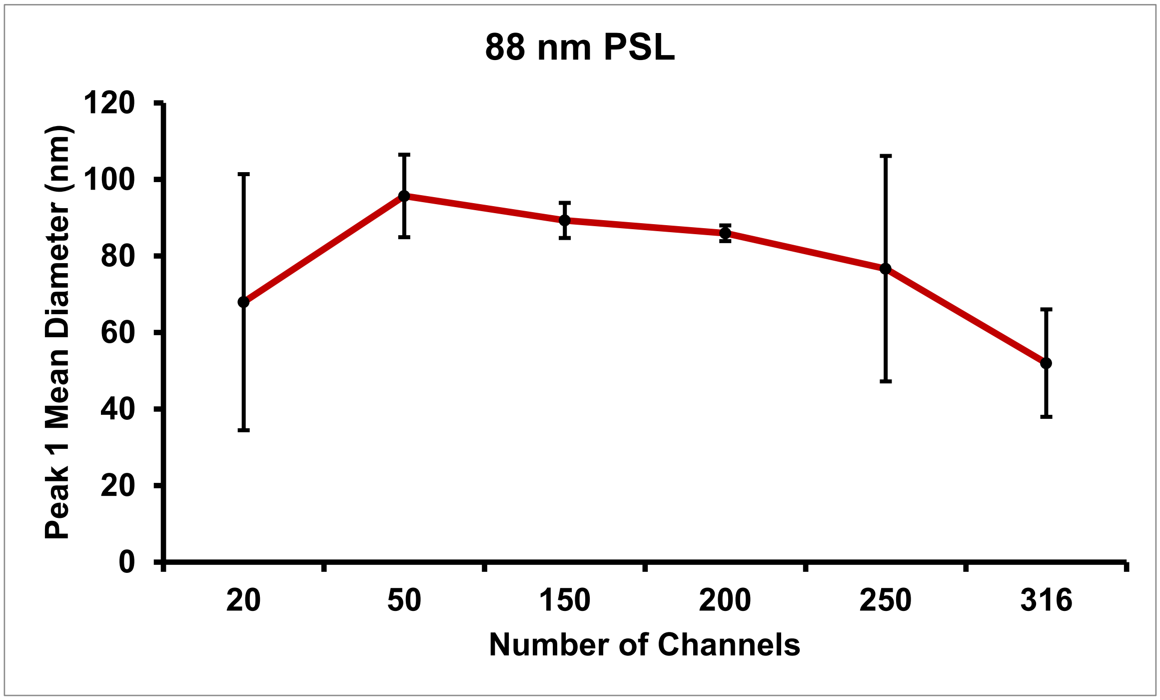

Figure 4: *Results of the mean diameter for peak 1 (88 nm PSL). Standard deviation is also plotted.*

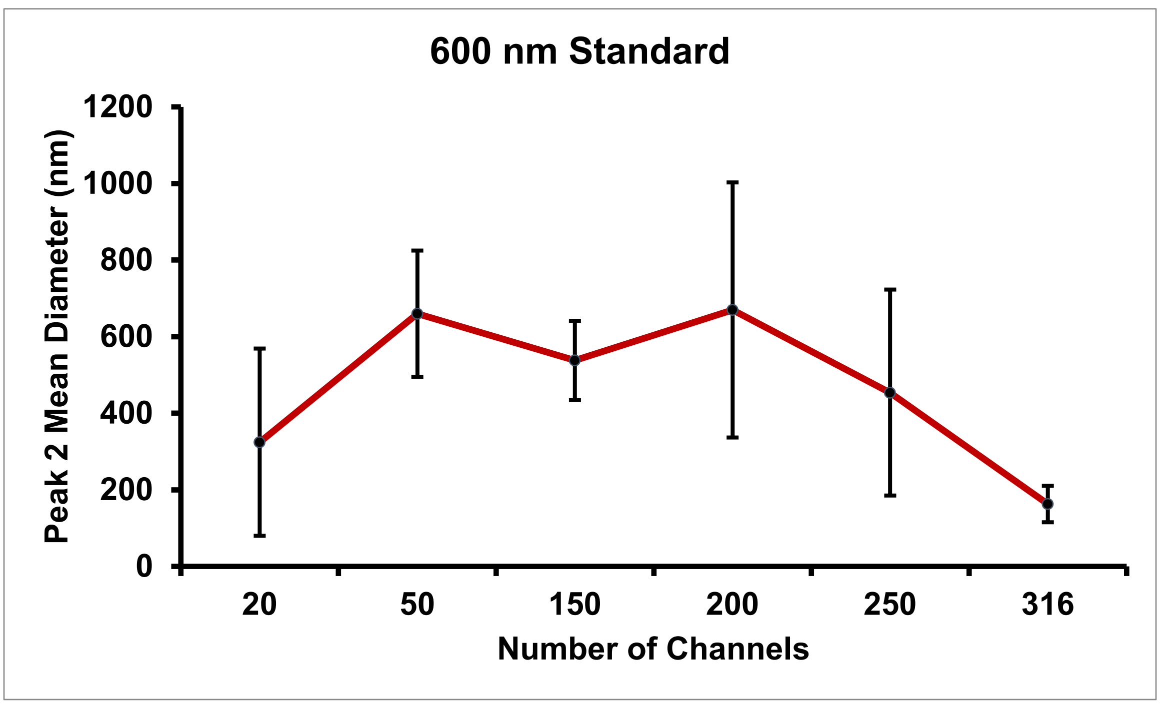

Figure 5: *Results of the mean diameter for peak 2 (600 nm PSL). Standard deviation is also plotted.*

The MSD graphs, which displayed the peaks of each replicate for all particle sizes in a sample, were obtained from each channels setting, **Figures 6-11**. The MSD graphs were plotted for peak intensity versus particle size, in diameter, for each replicate. Each color for the data plotted represented a single replicate.

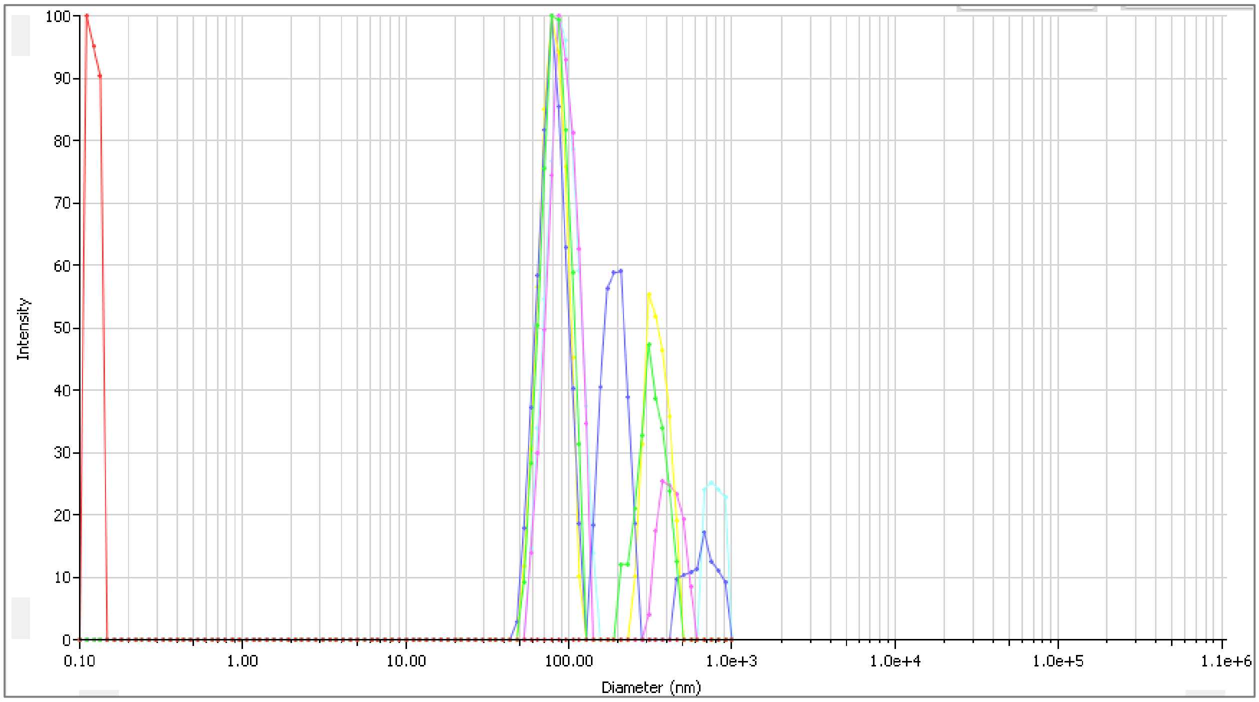

Figure 6: *MSD of sample containing 88 nm and 600 nm PSL particles measured with 20 channels.*

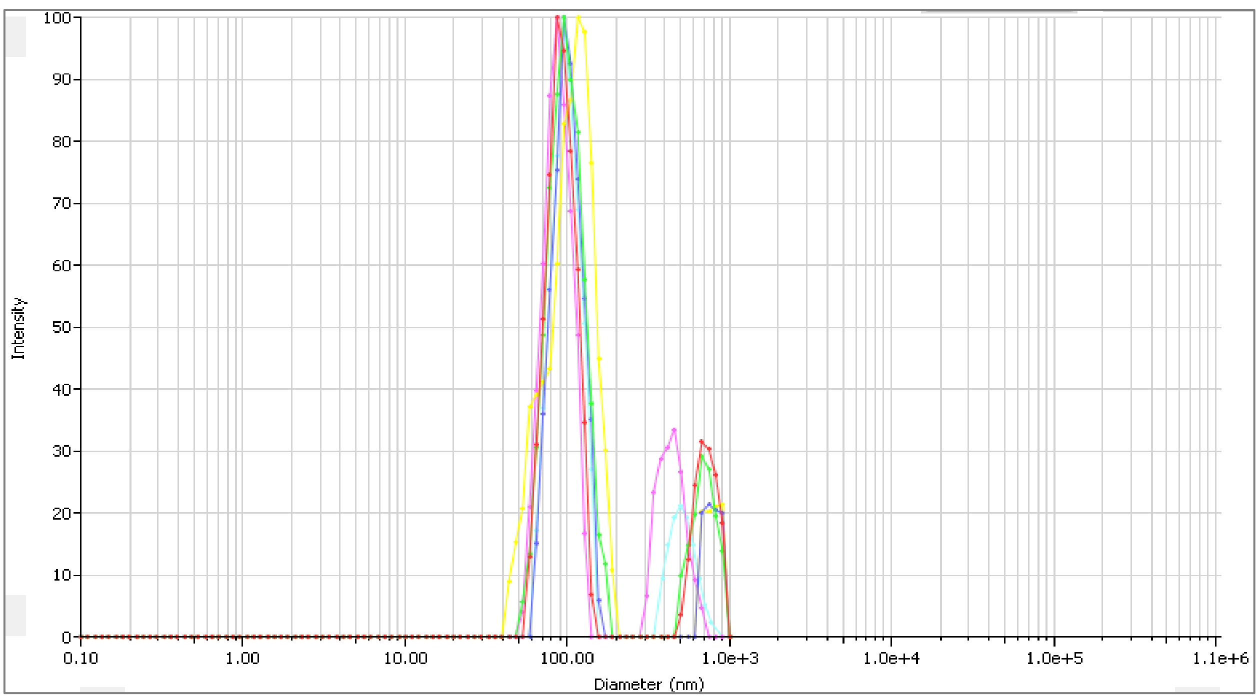

Figure 7: *MSD of sample containing 88 nm and 600 nm PSL particles measured with 50 channels.*

300 Innovative Way, Suite 222, Nashua NH 03062 USA
www.brookhaveninstruments.com
+1 (631) 758-3200

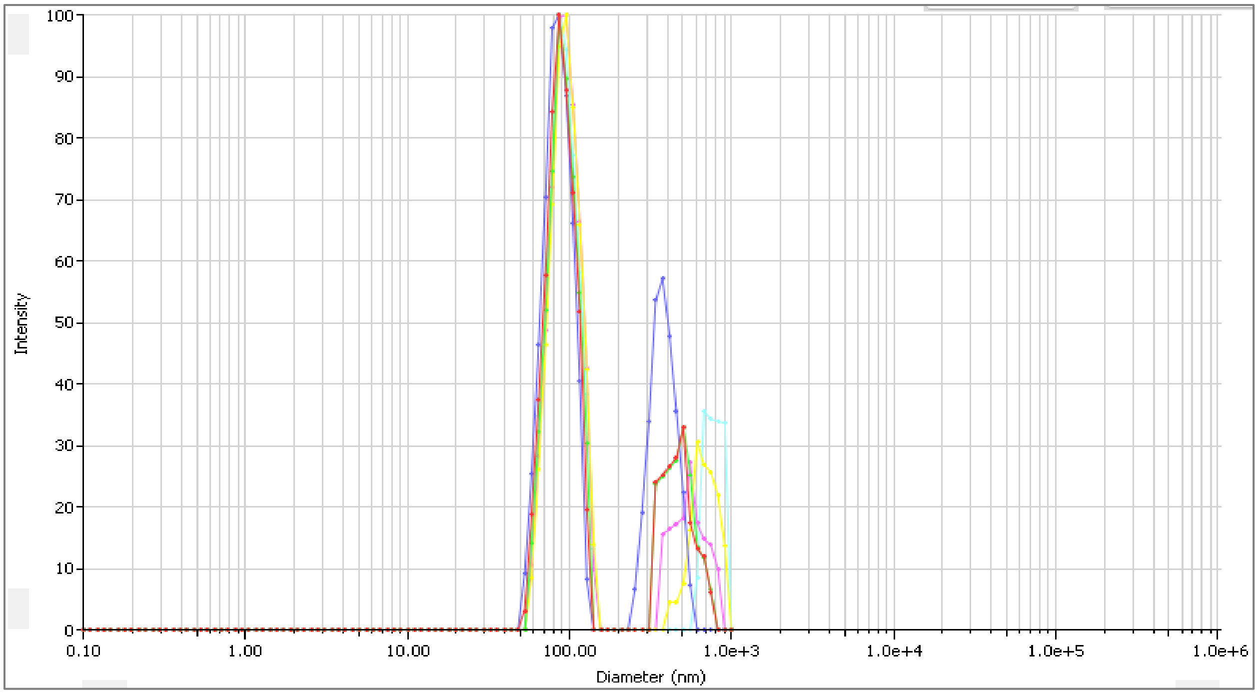

Figure 8: *MSD of sample containing 88 nm and 600 nm PSL particles measured with 150 channels.*

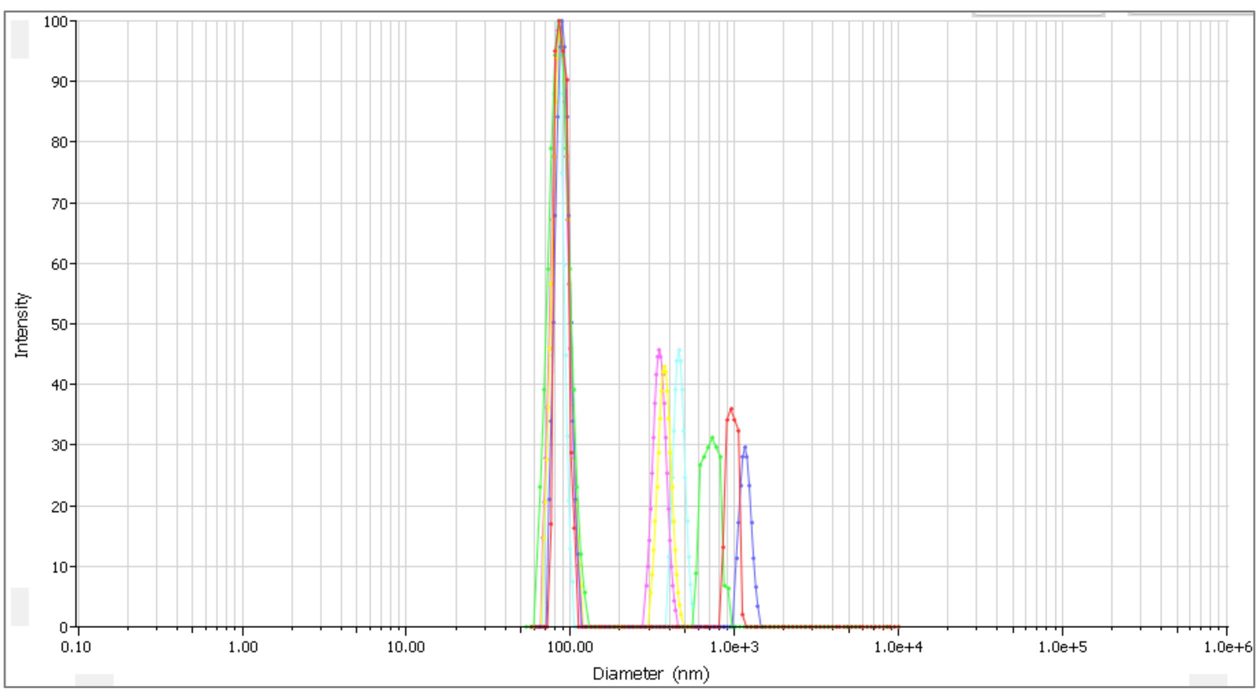

Figure 9: *MSD of sample containing 88 nm and 600 nm PSL particles measured with 200 channels.*

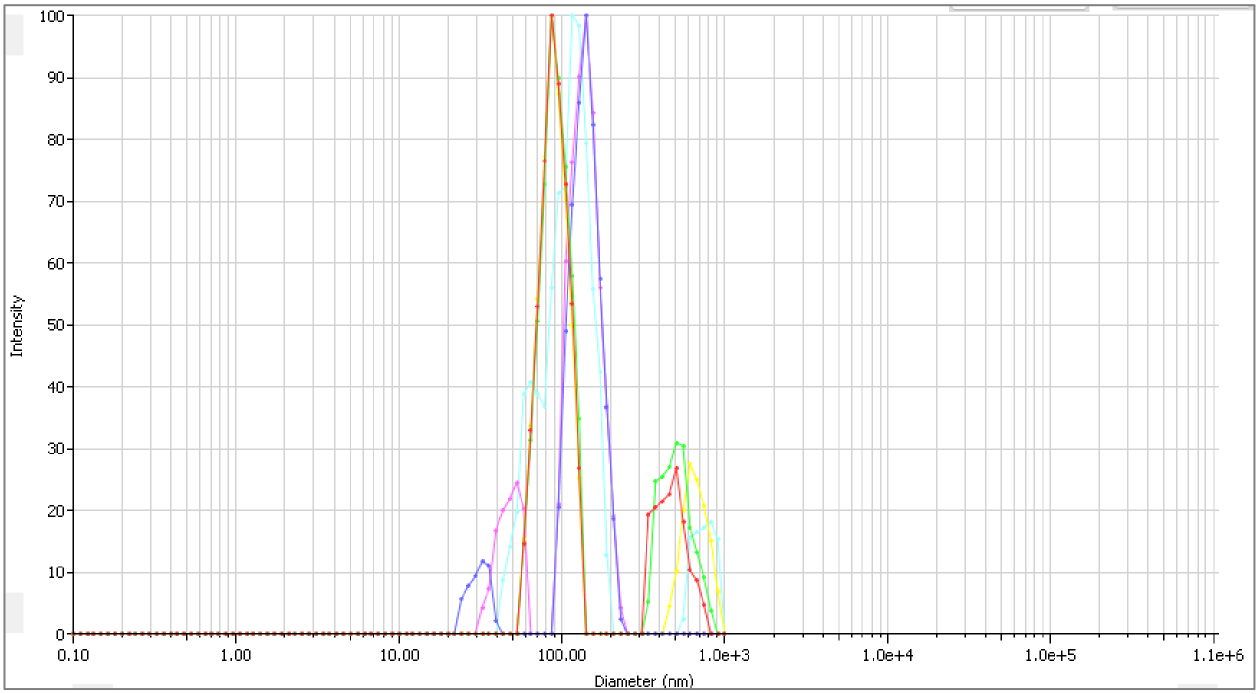

Figure 10: *MSD of sample containing 88 nm and 600 nm PSL particles measured with 250 channels.*

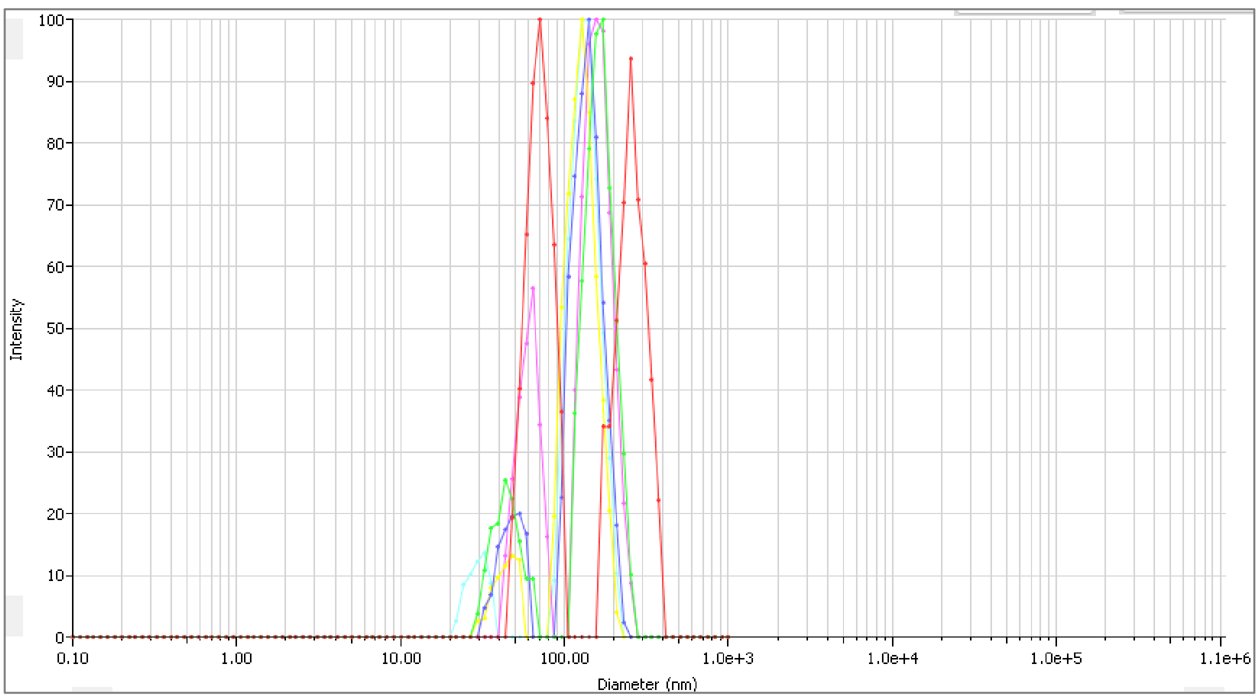

Figure 11: *MSD of sample containing 88 nm and 600 nm PSL particles measured with 316 channels.*

Figures 6, 10, and 11 presented MSD graphs with peaks that could not be distinguished from each other; however, The two peaks representing the two different particle size populations, were evidently seen in **Figures 7, 8, and 9.** Although Figure 10 did display two separate peak populations, peak 2 was not repeatable, as seen with the non-overlapping peaks for each replicate.

Polydispersity Index

Polydispersity index, PDI, is a useful measurement to determine if a sample is monodispersed or polydispersed. Lower PDI values such as values under 0.1 and closer to 0 represent samples that are monodispersed while values >0.1 represent polydisperse samples. **Table 3** displays the mean PDI results of the polydispersed 88 nm and 600 nm sample used for this study. The mean PDI values obtained at all the different channels settings represent a polydispersed sample.

Polydispersity Index Results						
Number of Channels	**20**	**50**	**150**	**200**	**250**	**316**
Mean Polydispersity Index	0.122	0.202	0.204	0.215	0.204	0.194
Standard Deviation	0.055	0.016	0.024	0.015	0.025	0.045

Table 3: *The polydispersity index (PDI) results for the 88 nm and 600 nm PSL particles obtained by changing the number of channels.*

Discussion

The aim of this study was to explore how the *channels* setting, a feature found in the new customizable correlator layout of Particle Solutions v4, influences the resolution of multiple particle size populations within a sample. This was achieved by preparing a polydispersed sample containing both 88 nm and 600 nm PSL particles. By utilizing the default 200 channels setting, First, the mean particle size diameter along with the respective standard deviation was determined for each sample population using the default setting of 200 channels.

Results depicted in **Tables 1, 2,** and **Figure 3**, revealed that while peak 1 can be clearly distinguished from peak 2, there is room for enhancing the repeatability of peak 2. Notably, the six replicates for Peak 1 demonstrated remarkable consistency with low variability in standard deviation, whereas those of peak 2 exhibited wider dispersion with higher variation resulting in a high standard deviation. At the default setting of 200 channels, peak 1 exhibited a low %RSD of 2.4%, contrasting with peak 2's high %RSD of 49.7%.

The second step was to determine if results could be optimized by performing the measurements using various channels below and above the default of 200, including: 20, 50, 150, 250, and 316 channels. **Table 1** demonstrated that the 200 channels was the optimal setting for the 88 nm PSL particles in the prepared sample, which resulted in a peak 1 mean diameter and standard deviation of 85.94 nm ± 2.05 nm and a %RSD of 2.4%. The optimal setting for peak 2, however, was 150 channels, which resulted in a peak 2 mean diameter and standard deviation of 537.77 nm ± 103.6 nm and a %RSD of 19.3%.

Results also indicated that the 20, 250, and 316 channels were not effective for measuring the different particle size populations in the sample. The expected peak 1 and 2 mean diameters and their respective standard deviations were not close to the expected particle sizes of 88 nm and 600 nm at all, as seen **in Table 1. Figures 6, 10, and 11** displayed peaks that were indistinguishable from each other.

The setting of 150 channels appeared optimal for both peak 1 and 2, with mean diameters and standard deviations of 89.29 nm ± 4.59 nm and 537.77 nm ± 103.6 nm, respectively, seen in **Table 1.** Furthermore, **Figure 8** displays two separate peaks with effective repeatability for the six replicates. Although 200 channels resulted in the lowest %RSD for peak 1 the impact on peak 2 resulted in a high standard error. By using 150 channels setting the %RSD was reduced from 49% using the default setting to 19.3 %. There was a slight increase in the %RSD for peak 1 but the increase to 2.4% was negligible compared to the decrease in %RSD for peak 2. Based on the results, it is determined that the setting of 150 channels is optimal for this sample.

The PDI, which determines if a sample is polydispersed or monodispersed, indicated that the sample being measured is a polydispersed sample, no matter how many channels were used.

The results of this study demonstrated that the number of channels *does* impact the resolution of multiple peaks as well as the repeatability of the results. It is important to note that DLS is not the most effective tool for measuring samples containing more than three different particle size populations. Since the optimal number of channels will vary from sample to sample, the most effective technique for determining the proper number of channels to use for your particular sample is to test channels above and below the default setting of 200 channels.

Conclusion

This study examined the channels feature of the new customizable correlator layout for DLS measurements using the Particle Solutions software. The purpose was to determine if modifying the number of channels in a DLS measurement would improve the resolution of different particle sizes in a single sample and of peaks found in the MSD graphs. Enhanced resolution results in accurate particle size measurements for different populations in a single sample, especially when these particles are close in size. To test the channels feature, a single sample containing 88 nm and 600 nm polystyrene latex particles diluted in 10 mM KNO_3 was prepared and measured at various channel settings including: 20, 50, 150, 200 (default), 250, 316 (highest possible with default first and last delays).

Based on the conducted experiments, it is determined that the number of channels does influence the resolution and distinguishability of multiple particle sizes and MSD graph peaks. Additionally, the repeatability of each peak is influenced by the number of channels as well. Results from this study indicated that the optimal number of channels lies for a mixture of 88 nm and 600 nm latex standard was 150, which is different from a pre-programmed setting of 200.

Particle Solutions v4 is the only DLS software in the market that allows the user to adjust the autocorrelation function. Particle Solutions v4 is used with the NanoBrook family of DLS and ZetaPALS instrumentation.

The latest release of Particle Solutions introduces the capability for the user to optimize correlator layouts. This ability is useful for difficult samples or otherwise unusual measurements.

Part 1: The New Customizable Correlator Layout – First Delay

Part 2: The New Customizable Correlator Layout – Last Delay

300 Innovative Way, Suite 222, Nashua NH 03062 USA
www.brookhaveninstruments.com
+1 (631) 758-3200