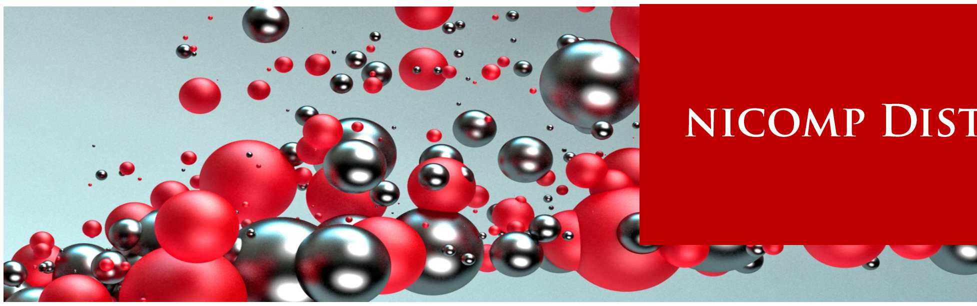


NICOMP DISTRIBUTIONS

TN–302

Technical Note

Nicomp DLS Intensity-, Volume-, and Number-weighted Gaussian Distributions

The Nicomp Model 380 measures particle size by detecting the scattered light (at a fixed angle) produced by an ensemble of particles suspended in solvent. The Intensity $I_s(t)$ fluctuates in time due to diffusion of the particles. There is a well defined characteristic lifetime of the *intensity fluctuations*, which is inversely proportional to the particle diffusivity. We computer the autocorrelation function C(t') of the fluctuating intensity $I_s(t)$, obtaining a decaying exponential curve in time. From the decay time constant τ, we obtain the particle diffusivity, D. Suing the Stokes-Einstein relation:

$$D=kT/6\pi\eta R$$

where k = Boltzmann's constant
η = viscosity of solvent (viscosity of water is 0.933×10^{-2} poise at 23°C)
T = temperature (°K = °C + 273)

We then compute the radius, R, assuming a sphere.

Since the autocorrelation function C(t') is constructed from the original scattered intensity value as a function of time, the quadratic fit and the corresponding Gaussian-like representation of the distribution of particle diffusivities (and, ultimately, diameters) reflect the fact that the D (diffusivities) contributions, or R (radius) contributions, are weighted by their corresponding scattering intensities.

There are six pieces of quantitative information contained in the summary display (Figure 1) of the Gaussian Analysis:

Intensity-weighted Mean: Mean Diameter: 219 nm

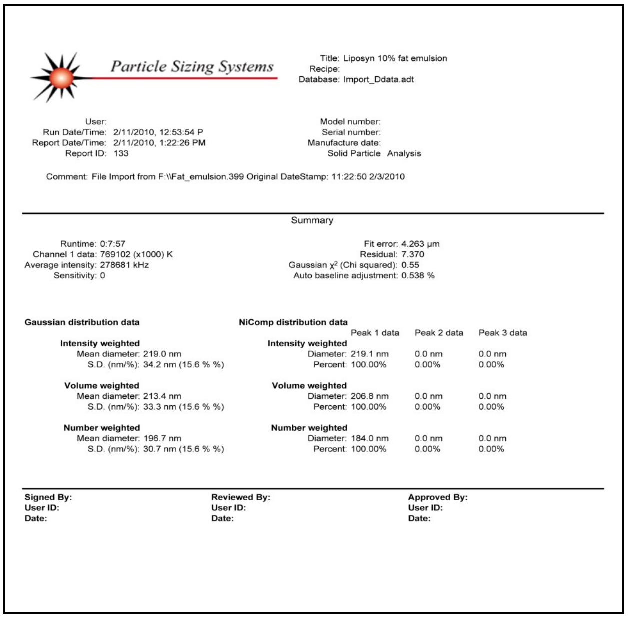
Width of the Distribution: Standard Deviation: 34.2 nm

Goodness of Fit: (Qualitative amount) Gaussian X^2 Chi Squared: 0.55

Aggregates of Dirt: Auto Baseline Adjustment: 0.538%

Actual Diffusion Coefficient: Mean Diffusion

Amount of Data Taken: Data



Particle Sizing Systems

Title: Liposyn 10% fat emulsion
Recipe:
Database: Import_Ddata.adt

User:
Run Date/Time: 2/11/2010, 12:53:54 P
Report Date/Time: 2/11/2010, 1:22:26 PM
Report ID: 133

Model number:
Serial number:
Manufacture date:
Solid Particle Analysis

Comment: File Import from F:\\Fat_emulsion.399 Original DateStamp: 11:22:50 2/3/2010

Summary

Runtime: 0:7:57
Channel 1 data: 769102 (x1000) K
Average intensity: 278681 kHz
Sensitivity: 0

Fit error: 4.263 μm
Residual: 7.370
Gaussian χ^2 (Chi squared): 0.55
Auto baseline adjustment: 0.538 %

Gaussian distribution data		NiComp distribution data	Peak 1 data	Peak 2 data	Peak 3 data
Intensity weighted		**Intensity weighted**			
Mean diameter:	219.0 nm	Diameter:	219.1 nm	0.0 nm	0.0 nm
S.D. (nm/%):	34.2 nm (15.6 % %)	Percent:	100.00%	0.00%	0.00%
Volume weighted		**Volume weighted**			
Mean diameter:	213.4 nm	Diameter:	206.8 nm	0.0 nm	0.0 nm
S.D. (nm/%):	33.3 nm (15.6 % %)	Percent:	100.00%	0.00%	0.00%
Number weighted		**Number weighted**			
Mean diameter:	196.7 nm	Diameter:	184.0 nm	0.0 nm	0.0 nm
S.D. (nm/%):	30.7 nm (15.6 % %)	Percent:	100.00%	0.00%	0.00%

Signed By: **User ID:** **Date:**
Reviewed By: **User ID:** **Date:**
Approved By: **User ID:** **Date:**

Figure 1: Summary of the Gaussian Distribution

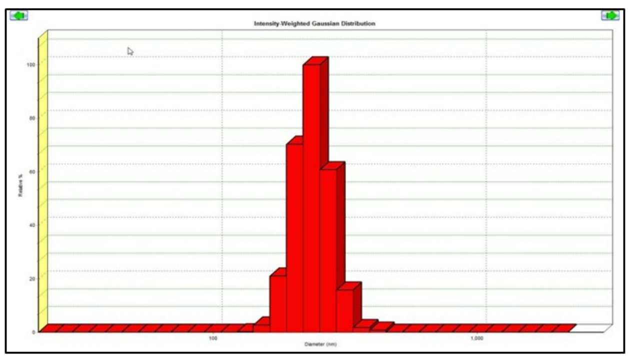


Figure 2: Intensity-weighted Gaussian Distribution

The problem is the value of the Mean Diameter is intensity-weighted. Most users do not care which particle contributed the most scattering, intensity. What they would like to know is what size contributes the most volume, volume-weighted or where the largest population of particles is located, number-weighted.

First, let us look at the simplest case: the Raleigh region. This is defined where the particle diameter is much less than τ, the wavelength of light (typically < 150 nm). The particles scatter light as point scatterers (equal in all directions).

Let us determine the behavior between intensity-, volume -, and number-weighted by reviewing the relationship between particle size and scattering intensity. For particle sizes much smaller that the wavelength of light (< 150 nm) you are in the Raleigh region where:

$f(n_p n_s) \times (Mw)^2 \times I_o$ or
$I_s = g(n_p n_s) \times V^2 \times I_o$
where n_p = is the index of refraction of the particle
n_s = is the index of refraction of the solvent
I_o = laser intensity

And where the contribution C(t') of particle decaying exponential, corresponding to a given diameter, d_i, should be weighted by the factor $N_i(Vi)^2$ where N_i is the number of particles having diameter, d^i, and V_i is their individual volume, which is proportional to $(di)^3$.

Hence, each diameter "slice" of the intensity-weighted distribution (Figure 2) has associated with it this factor $N_i d_i^6$.

$$\text{Intensity-weighted } \alpha\ N_i V_i^2 \text{ or } N_i d_i^6$$

To convert this to a volume-weighted (Figure 3) distribution we remove a factor of V_i or d^3 from each slice of the distribution.

$$\text{Volume-weighted } \alpha\ N_i V_i^3$$

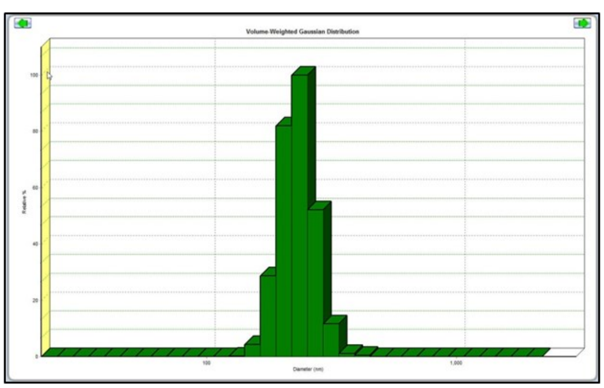


Figure 3: Volume-weighted Gaussian Distribution

We perform one additional division of Vi to obtain the number-weighted distribution:

$$\text{Number-weighted } \alpha\ N_i$$

For sizes larger than 150 nm, the rules of Mie scattering take effect when intra-particle interference effects become important.

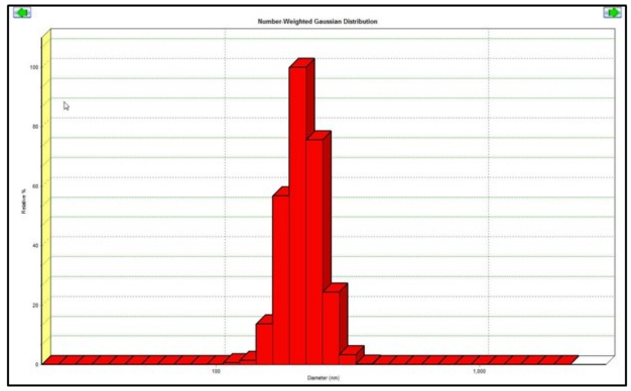


Figure 4: Number-weighted Gaussian Distribution

The Nicomp uses the "rules" of light scattering making corrections for Mie scattering. In order to obtain the volume- and number-weighted plot distributions from the intensity-weighted plot the relationships are as follows:

$$\text{Intensity-weighted } \alpha\ N_i V_i^2 G_i$$
$$\text{Volume-weighted } \alpha\ N_i V_i G_i$$
$$\text{Number-weighted } \alpha\ N_i G_i$$

where G is a factor that varies between unity and zero depending on the particle size, laser wavelength, and angle of detection.

That is why there are some cases in larger particle size distributions where the volume-weighted mean diameter is larger than the intensity weighted mean.

Also keep in mind, the amount that the mean diameter of the distribution shifts depends on the width of the intensity-weighted distribution. An extreme case is where you have a mono-sized peak; the intensity-, volume- and number-weighted means would all be the same.

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Particle Sizing Systems

Building solutions one particle at a time.