

[Polydispersity] supplementary to {§14.8.3:471}

One of the effects of polydispersity is smearing of the SANS data, such as smoothing the oscillations introduced by the form factors. The commonly used size distribution functions are first, the *Gaussian distribution*

$$D(R; \bar{R}, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(R - \bar{R})^2}{2\sigma^2}\right], \quad (1)$$

where σ is the half-width of the Gaussian function. Second, the *log-normal distribution*

$$D(R; \mu, \sigma) = \frac{1}{\sigma R\sqrt{2\pi}} \exp\left[-\frac{(\ln R - \mu)^2}{2\sigma^2}\right], \quad (2)$$

where $\mu = \ln(R_{med})$. Unlike the Gaussian distribution, which is symmetric with respect to \bar{R} , the log-normal distribution is skewed to the low- R side. The physical meaning of μ and σ is not as obvious as the corresponding Gaussian variables. It requires a “back transformation”: $\mu \rightarrow \exp(\mu)$, $\sigma \rightarrow \exp(\sigma)$, in order to compare with the Gaussian distribution. The difference between the two distributions hinges on whether additivity (Gaussian) or multiplication (log-normal) is the basis for decision making. The log-normal distribution proves to be applicable to naturally occurring phenomena across many scientific disciplines. It can be shown that the log-normal distribution reduces to the Gaussian distribution when $\sigma \ll \ln(\mu)$.

And third, the *Schulz distribution*

$$D(R, R_{av}, z) = (z+1)^{z+1} \left(\frac{R}{R_{av}}\right)^z \frac{\exp\left[-(z+1)\frac{R}{R_{av}}\right]}{R_{av}\Gamma(z+1)}, \quad \text{for } z > -1. \quad (3)$$

In (3), $\Gamma(z) = \int \exp(-t)t^{z-1} dt$ is the gamma function, and the standard deviation is $\sigma = \frac{\bar{R}}{\sqrt{z+1}}$.

This distribution was first used to represent the molecular weight distribution of synthetic polymers.