

Supporting information for 'The Downside of Dispersity: Why the Standard Deviation is a More Intuitive Measure of Dispersion in Precision Polymerization'

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Derivation of the expression for dispersity in terms of standard deviation and mean.

In a polymer molecular weight distribution, in which x is the degree of polymerization, and $f(x)$ is the frequency of chains of length x , normalized such that $\sum f(x) = 1$, the number and weight average degrees of polymerization DP_n and DP_w are defined as follows:

$$DP_n = \mu = \frac{\sum xf(x)}{\sum f(x)}$$
$$DP_w = \frac{\sum x^2f(x)}{\sum xf(x)}$$

Their ratio gives the dispersity, \mathfrak{D} :

$$\mathfrak{D} = \frac{DP_w}{DP_n} = \frac{\sum x^2f(x) \cdot \sum f(x)}{(\sum xf(x))^2}$$

The standard deviation, σ , is defined as the root mean square difference from the mean, giving:

$$\sigma^2 = \sum (x - \mu)^2 f(x)$$

Expanding the sum gives:

$$\sigma^2 = \sum x^2f(x) - 2\mu \sum xf(x) + \mu^2 \sum f(x) = \sum x^2f(x) - \mu^2$$

This is the well-known expression for the variance as the mean of the squares minus the square of the mean.

Substituting this formula into the expression for \mathfrak{D} gives:

$$\mathfrak{D} = \frac{DP_w}{DP_n} = \frac{\mu^2 + \sum x^2f(x) - \mu^2}{\mu^2} = 1 + \frac{\sigma^2}{\mu^2}$$

