TECHNICAL NOTE

Atomic Absorption

Atomic Absorption Calibration Algorithms

For proper instrument and method validation, the calibration algorithms (calculation equations) used by the instrument firmware or software frequently must be known. Documentation on the equations used with PerkinElmer® atomic absorption instrumentation for linear calibrations (calculated intercept) are shown below:

For the line: $y = mx + b$

$$\text{slope } (m) = \frac{(n)\,\Sigma\, x_i\, y_i - \Sigma\, x_i\, \Sigma\, y_i}{(n)\,\Sigma\, x_i^2 - (\Sigma\, x_i)^2}$$

$$\text{intercept } (b) = \frac{\Sigma\, x_i^2\, \Sigma\, y_i - \Sigma\, x_i\, \Sigma\, x_i\, y_i}{(n)\,\Sigma\, x_i^2 - (\Sigma\, x_i)^2}$$

$$\text{correlation coefficient } (r) = \frac{(n)\,\Sigma\, x_i\, y_i - \Sigma\, x_i\, \Sigma\, y_i}{\left[\sqrt{(n)\,\Sigma\, x_i^2 - (\Sigma\, x_i)^2}\right]\ \left[\sqrt{(n)\,\Sigma\, y_i^2 - (\Sigma\, x_i)^2}\right]}$$

where x_i is the concentration, y_i is the absorbance and n is the number of standards.

Please note that the point 0,0 is included in the calculations.

The multiple correlation coefficient (r) for the nonlinear calibration curve is calculated as shown below. Note that the calculation requires that you already know the nonlinear equation coefficients, since you must calculate the estimated concentration at each concentration point.

PerkinElmer®
For the Better

$$r = \sqrt{1 - \frac{\text{Residual Variance}}{\text{Variance of Concentration}}} = \sqrt{1 - \frac{\sum_{1}^{n} (C - \hat{C})^2}{\sum_{1}^{n} (C - \bar{C})^2}}$$

where n is the number of standards, C is the entered concentration, $\hat{C}$ is the calculated concentration and $\bar{C}$ is the average entered concentration:

$$\bar{C} = \frac{\left[\sum_{1}^{n} C\right]}{n}$$

The nonlinear calibration equation is:

$$C = k_0 \left[\frac{k_3 A^2 + k_1 A}{k_2 A - 1}\right]$$

The equations used to calculate standard deviation (SD) and precision (rsd) for both linear and nonlinear calibrations are:

$$SD = \sqrt{\frac{\sum (x_1 - x_{mean})^2}{n - 1}}$$

$$rsd\ (\%) = 100 * \frac{SD}{mean}$$

Where x_i is each replicate measurement, x_{mean} is the mean value and n is the number of measurements.

The above calculations are all performed using the original data, before any rounding operations, carried to 8 digits.

PerkinElmer, Inc.
940 Winter Street
Waltham, MA 02451 USA
P: (800) 762-4000 or
(+1) 203-925-4602
www.perkinelmer.com

PerkinElmer®

006987A_01