

Protein heterogeneity in wheat lots Quantification of sampling and analytical errors

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Purpose: An in depth heterogeneity analysis of wheat lots from various field experiments with respect to protein concentration was conducted in order to quantify and compare both sampling and analytical errors as defined by the theory of sampling (TOS) (Gy, 2004).

Methods: In all, thirty wheat samples of forty-two seeds were extracted from three different wheat lots. Half of these were purposely extracted incorrectly by using a spoon, while the other half was extracted correctly by using a riffle splitter.

The protein content of every single seed was determined by near-infrared transmission (NIT) spectroscopy in connection with partial least squares regression (PLS-R). The variance of the global estimation error (GEE) was estimated as well as its additive contributions; the fundamental sampling error (FSE), the grouping and segregation error (GSE), the incorrect sampling error (ISE) and the total analytical error (TAE), i.e.

$$\sigma^2(\text{GEE}) = \sigma^2(\text{FSE}) + \sigma^2(\text{GSE}) + \sigma^2(\text{ISE}) + \sigma^2(\text{TAE}).$$

Results: The GEE variance of the spoon extractions was eighty percent higher than that of the riffle splitter extracted samples. In addition the sampling variances of FSE, GSE and ISE were all in the same order of magnitude and each approximately ten times higher than the TAE variance.

Conclusions: The applicability of TOS to quantify and evaluate the various error contributions to the overall estimation of the protein concentration was confirmed. The variances of the errors generated by the sampling processes (both correct and incorrect) were an order of magnitude higher than the variance of the analytical error and thus stress the need for proper sampling in chemometrics, process analysis and in chemistry as such.