What is the Uncertainty Factor?

Introduction

The uncertainty of a measurement result is often as important as the measured quantity value itself, as it controls what decisions can be made using that result, such as regulatory compliance. Appropriate expression of the measurement uncertainty (MU) is crucial, and there are situations when the traditional, symmetric, expanded uncertainty interval is not sufficient. This leaflet aims to explain the concept of the uncertainty factor and how it can be used to provide a convenient and realistic uncertainty interval in particular circumstances.

Ways of expressing measurement uncertainty

Many laboratories now estimate measurement uncertainty and usually express it as either expanded uncertainty (U), or relative expanded uncertainty (U'), typically with a coverage factor (k) of two for approximately 95 % confidence. The measurement result is then expressed as $x \pm U$ (where x is the measurement quantity value, and $\pm$ is 'plus-minus'). The range of values that contains the value of the measurand (i.e. the true value of the analyte concentration) is then between $x - U$ and $x + U$ with approximately 95 % confidence. An example of this would be for a measurement result of 50 $\pm$ 5 mg kg^{-1}, where the value of the measurand is believed to lie between 45 and 55 mg kg^{-1}. This approach works well generally, unless the value of MU is high (e.g. the relative standard uncertainty u' is over 20 %), or the frequency distribution of repeated measurements is positively skewed, rather than the usual Gaussian (i.e. Normal) shape. In these situations, the expanded uncertainty factor (^{F}U) is a more useful way to express the MU, and the measurement result is expressed as x $^{x}/$ ^{F}U (k = 2, where '$^{x}/$' is called 'times-over'). In the previous example, but with much larger MU expressed as an uncertainty factor of ^{F}U = 2.0, the uncertainty interval 50 $^{x}/$ 2.0 is from 25 (i.e. 50/2) to 100 (50 x 2) mg kg^{-1}, which is clearly an asymmetric confidence interval.

How is the uncertainty factor calculated? - A case study

One example of the calculation of ^{F}U is for the determination of lead at a contaminated land site, and includes the MU arising from the primary sampling of the top soil. A detailed description is given elsewhere [1], but the key issues are that 100 sampling targets were sampled in a grid across the site and sent for the determination of Pb by ICP-AES after acid digestion, in a competent laboratory. The MU was estimated using the 'duplicate method' ([1] p17-19), in which 10 randomly selected targets had duplicate samples taken, that were both analysed twice, giving 40 measurement results.

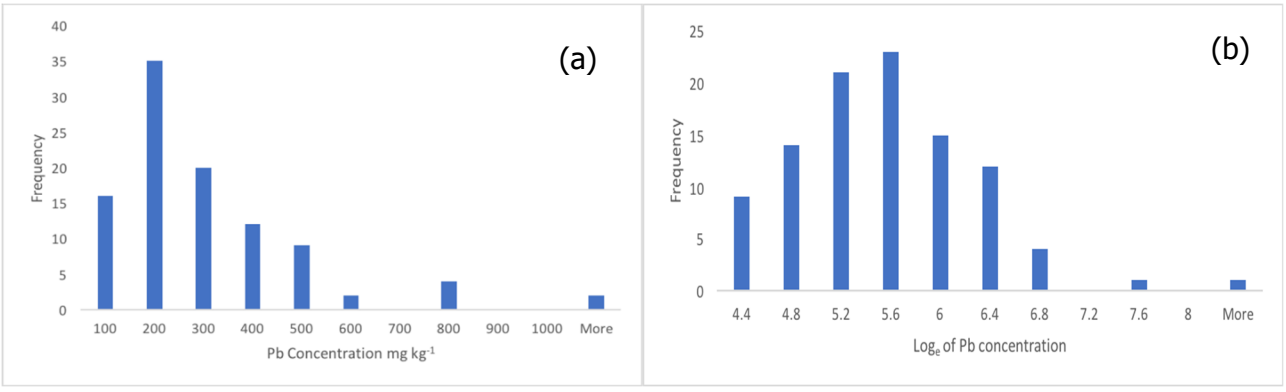

Figure 1. Histograms of the Pb concentration (as mass fraction in mg kg^{-1}) measured in 100 soil samples shown on (a) the original linear scale (b) after natural logarithms were taken

In this case the MU was estimated only as the repeatability standard deviation, which was the main source of uncertainty. The analytical bias was checked by analysing CRMs and found to be negligible.

When the MU is expressed as U', it is calculated from the standard deviation (s_{meas}) of a measured quantity value (x), typically using $k = 2$ for approximately 95 % confidence, with the equation

$$U' = 100\frac{2s_{meas}}{x}\% \qquad \text{Equation 1}$$

The validity of this equation assumes that the frequency distribution of the replicated measurement results is Gaussian. However, if this distribution is shown to be positively skewed (Fig 1a)*, it may well be lognormal. This can be confirmed by taking natural logarithms of all of the measurement results, $\ln(x)$ or $\log_e(x)$, and determining if this then gives a near-normal distribution (Fig 1b).

The uncertainty factor ${}^{F}U$ can be calculated from the standard deviation ($s_{L,meas}$) of these 40 log-transformed measurement results, produced by applying the 'duplicate method', using

$${}^{F}U = exp(2s_{L,meas}) = e^{2s_{L,meas}} \qquad \text{Equation 2}$$

For practical purposes, ${}^{F}U$ can be calculated by inputting the original 40 measurement results into a software package that applies Analysis of Variance (ANOVA), e.g. [2]. For this example, the value of ${}^{F}U$ was calculated as 2.62, and it is applicable over the range of concentration represented by the duplicates. For a typical single measurement result of 300 mg kg^{-1}, the value of the measurand would lie, therefore, between 115 (300/2.62) and 784 (300 x 2.62) mg kg^{-1}. This wide and asymmetric confidence interval is mainly caused by uncertainty from the sampling process, due to the high level of heterogeneity of the Pb distribution in the soils within each sampling target.

Broader implications

High levels, and asymmetric distributions, of uncertainty can also arise in the analytical part of the measurement process. For example, in one study on the determination of genetically modified organisms (GMO) in soya [3] (Fig 2), the distribution suggests that ${}^{F}U$ could be the most applicable way to express MU in some purely analytical systems, as well as for those dominated by uncertainty from sampling. In such situations, ${}^{F}U$ can be calculated using Equation (2), without the need for ANOVA.

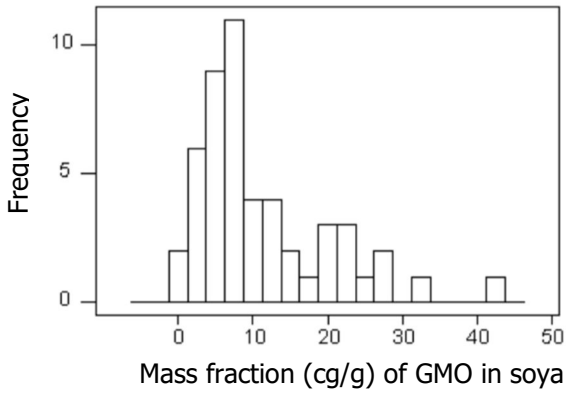

Figure 2. Log-normal distribution of proficiency test measurements of GMO in soya [3]

Communication of MU

One challenge in using ${}^{F}U$ to express MU is to communicate its meaning clearly to the user of the measurement results. The statement of a measurement result can take the form x ˣ/ ${}^{F}U$. Hopefully, this leaflet will be one way to assist in communicating the meaning of a result expressed in this form.

More information / further reading

[1] Ramsey M. H., Ellison S. L. R. and Rostron P., (eds.) Eurachem/EUROLAB/CITAC/Nordtest/AMC Guide: *Measurement uncertainty arising from sampling: a guide to methods and approaches.* Second Edition. Example A2, p44-52. Eurachem (2019) ISBN 978 0 948926-35-8. Available from http://www.eurachem.org.

[2] RANOVA3, available from https://www.rsc.org/membership-and-community/connect-with-others/through-interests/divisions/analytical/amc/software/.

[3] AMC (2004) GMO Proficiency testing: Interpreting z-scores derived from log-transformed data Technical Brief No 18 https://www.rsc.org/images/GMO-proficiency-testing-technical-brief-18_tcm18-214857.pdf.

*In this example (Fig. 1) the distribution is from 100 different sampling targets. The positive skew is caused by the heterogeneous distribution of the analyte at that scale. This heterogeneity is also likely to apply at the smaller scale within each sampling target, which is reflected in the estimate of MU.

The Analytical Methods Committee

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