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Manifestation of Sources of Uncertainty in Measurements

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Abstract: This article highlights the inaccuracies that appear in measurement results and their sources. Methods for estimating uncertainty and an analysis of the steps that need to be taken to assess the uncertainty inherent in the measurement result are presented.

KeyWords: uncertainty, size, measurement, parameter, evaluation methods, standard uncertainty, source.

Uncertainty is a relatively new concept such as the qualitative characteristics of measurement results. The traditional terms previously used in metrology are "error" and "error analysis". This requires a simple comparison of measurement results across countries. This method must be so versatile that it can be used for any type of measurement; when estimating uncertainty, "description of the size of the measurement" requires not only expressing the exact measurand, but also quantifying the size of the measurement. related to its parameters [1-3].

Type A (uncertainty) estimation: A method for estimating uncertainty through statistical analysis of a series of observations.

In most cases, the measured quantity Q_u is not a simple measured quantity, it is another quantity Q_1 , Q_2 ,

 Q_n depends on the measured quantities, $Q_u=f(Q_1, Q_2, ..., Q_n)$, and accordingly the concept of standard uncertainty is introduced. If Q_1 , Q_2 , ..., Q_n are independent (unrelated) quantities, then the cumulative standard uncertainty is expressed as follows:

$$U_i^2 = \sum_{i=1}^n \left(\frac{\partial Q_U}{\partial Q_i}\right)^2 u_i^2$$
^[1]

Here U_i^2 - are the standard uncertainties estimated for each type A and B.

The following formula is used to estimate uncertainty for Type A:

$$U_A = s(Q) = \sqrt{\frac{\sum_{i=1}^{n} (Q_i - \bar{Q})^2}{n-1}},$$
[2]

Where Q_i – independent (unrelated) values for repeated observations; Q – arithmetic mean; n is the number of observations.

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The type of uncertainty estimate is called standard deviation, or simply type A standard uncertainty. Type B (uncertainty) estimation: A method of estimating uncertainty using methods that differ from statistical analysis of a series of observations. The uncertainty estimate for Type B is based on the law of equal distribution of the most commonly used probabilities: if there is where b_1 , b_2 – boundary fractions of the quantity obeying the law of equal distribution. Coverage factor (k): coefficient expressed by a number used as a factor of the final standard uncertainty to achieve total uncertainty: $U = k \cdot u_s$, in which case the measurement result is expressed as $Q = q \pm U$ [5-8].

Such an interval may be in the following range $q-U \le Q \le q+U$, and it is generally assumed that the coverage factor is between two and three. The following steps should be taken to estimate the uncertainty inherent in any measurement result.

Step 1. Describe the quantity measured.

It is necessary to clearly state what is being measured by entering the relationship between the measured quantity and the parameters associated with it (eg measured quantities, constants, reference values for assessment, etc.). If possible, adjustments are made to some of the systemic effects. Such descriptive information is usually provided in an appropriate method document or other method description.

Step 2. Identify sources of uncertainty.

A list of sources of uncertainty has been compiled. It includes sources that contribute to parameter uncertainty in the same proportions as defined in step 1, but may also include other sources of uncertainty, such as those derived from chemical assumptions.

Step 3. A quantitative description of the components of uncertainty.

The uncertainty value specific to each identified potential source is determined and estimated. It is often possible to estimate or identify a single contribution of uncertainty associated with multiple sources. It is also important to consider that the available data adequately account for all sources of uncertainty and that additional experiments and studies need to be carefully planned to ensure that all sources of uncertainty are adequately accounted for [9,10].

4-step. Calculation of the final uncertainty.

The information obtained in step 3 consists of a number of quantified properties that are subject to general uncertainty or are associated with individual sources or with end-effects (effects) of several sources. These properties need to be expressed as standard deviations and combined to obtain the final standard uncertainty in accordance with current rules. An appropriate coverage factor should be used to obtain the expanded uncertainty.

Typical sources of uncertainty:

1. Sample selection.

In cases where sampling processes carried out in the laboratory or directly at the object of analysis are part of the analytical method, effects such as random differences between samples and any possibility of bias (bias) in the sampling process form the final uncertainty.

2. Storage conditions for samples.

If the measured (tested) samples are stored for some time before measurements are taken, the storage conditions may affect the result. Consequently, storage duration as well as storage conditions should be considered sources of uncertainty.

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3. Hardware effects

Such effects, for example, limit the accuracy of analytical balances; the presence of a thermostat capable of maintaining an average temperature different from the fixed one (within the specified limits); may include an automatic analyzer that may be subject to overload effects.

4. Purity of reagents.

Even if the original reagent is tested, the concentration of the titration solution cannot be determined with absolute precision due to some uncertainty associated with this test method. Many reagents, such as organic dyes, are not considered 100% pure and may contain isomers and inorganic salts. At the very least, the purity of such substances should be specified by the manufacturer. Any assumptions about the level of cleanliness involve an element of uncertainty. Deviations from the expected stoichiometry or incomplete reaction or auxiliary reactions may be necessary in cases where it is assumed that the analytical process obeys the specified stoichiometry.

5. Measurement conditions.

For example, a bulk glass container can be used at a temperature other than the calibrated temperature. Consideration should be given to large corrected temperature effects, but even so, any uncertainty in liquid and glass temperatures should be considered. Likewise, if the materials used are sensitive to possible changes in humidity, ambient humidity can make a difference.

6. Sample effect

The composition of a complex matrix can affect the removal of a detected component or the response (display) of the instrument. Sensitivity to the form of detection of the detected component can exacerbate this effect.

The stability of the sample or detectable component may change due to changes in thermal conditions or photolytic effect during analysis.

7. Computational effects

Selecting an incompatible model during ranking, such as using linear classification in a non-linear response, results in very poor agreement and greater uncertainty. Removing and rounding numbers can lead to inaccuracies in the final result. Since these situations are difficult to predict, some uncertainty may be justified.

8. Correction to the blank sample.

Some uncertainty in the value of the blank correction is equally consistent with skepticism about the need for this correction. This is especially important when analyzing traces.

9. Operator effect

Possibility of recording low or high readings of measuring instruments.

Possibility of minor differences in the interpretation of the method.

10. Random effects

Random effects lead to inaccuracies in all definitions. Of course, this item should be included in the list of sources of uncertainty.

For most reference materials (SN), especially SN certified by interlaboratory experiments, it makes more sense to use the concept of uncertainty as a metrological characteristic than the concept of error. For example, MVN Analytical Ltl (UK) has its own description DSN 03.0305: 2004 SN Uncertainty. The

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certificate indicates the expanded uncertainty of some \mathbb{R} reliability probability and (K) coverage factor. For example, SN DSN 03.0241: 2004, issued by Raragon Scientific Ltd (England), has expanded uncertainty with a reliability probability R= 95% and a coverage factor K = 2. The expanded uncertainty is stated on the certificate without specifying the coverage factor at any reliable probability \mathbb{R} . For example, SN from Petrolet Analyzer Corporation Gmbn (Germany) "(S_(p)) – reliable probability \mathbb{R} for the method with standard deviation – expanded uncertainty of the mean value obtained with the participation of laboratories (n)". Direct comparison of the characteristics of error and uncertainty is not accurate, therefore, as a rule, $U = (t \cdot S_{(p)})/\sqrt{n}$ the statistical estimates of these metrological instruments are compared. If a standard or final uncertainty is given, then the standard deviations of their estimates are appropriate:

$$\Sigma(A) = u(A) \text{ or } \sigma(A) = u_c(A)$$
 [3]

where u(A) and $u_c(A)$ are the corresponding standard and final uncertainties in determining the certified SN value; A - is the certified SN value; $\sigma(A)$ - is the standard deviation of the certified SN value, then the standard deviation of its value is appropriate.

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