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Calculation of measurement uncertainty

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Abstract
Calculation of measurement uncertainty is the basis of measurements, tests in calibration laboratories, tests and their calibration, tests reports. Calculation of measurement uncertainty is one of the basic requirements of the international standard ISO/IEC 17025 General requirements for the competence of testing and calibration laboratories, on the metrological traceability of measurements. Calculation of measurement uncertainty has a direct impact on the development of trade and technology, the production and marketing of certain products in the measurement chain with a high degree of accuracy. The measurement uncertainty is calculated and defined as a value, accompanied by the result of a measurement, a test that is characterized by the distribution of values that can reasonably describe a measurement.

Keywords: Standard, Uncertainty, Error, Deviation, Traceability

1. Introduction

In everyday life, we are often faced with a variety of measurements from ordinary household purchases such as: tomatoes, potatoes, peppers, bananas, flour, rice, car fuel and other products such as clothing, underwear and we will always have some kind of measurement whether that is their mass, length, volume or something else. While these measurements may seem very usual, when buying or selling products with greater sensitivity such as: carbohydrates, proteins, vitamins or different types of medicaments, giving doses with defined concentration as well as their use according to the instructions of different specialists, use of different chemicals, herbicides, etc., the problem that arises stands in the dilemma that which is the real amount of the component that we need for food, treatment and other aspects of the use of those substances that we are measuring.

The question that always arises in our minds is whether the quantity we have measured is true or not, and if not, what is the difference between the given quantity and the real one? What is the error in measurement? Likewise, many other questions arise on the spot, and in metrological terms we have called this concept “uncertainty in measurement”.

From that we conclude that the objective of a measurement is to determine the value of the component we are measuring, i.e., the specific quantity to be measured. When these measurements apply to a particular test, the general term measurement may cover different measurements, e.g., the strength of a material, the concentration of an analyte, the level of noise or radiation emission, the number of microorganisms, et cetera.

Starting from the principle of relativity, "everything is relative" as well as the fact that all measurements are realized through various physical, chemical, electrical comparisons, etc., a measurement always starts with a proper specification of the measurement device, generic measurement method and specific detailed measurement procedure.

Many scientists often ask the question, do we actually have accurate measurements? The answer always comes out as: Accurate measurement is an abstract term!

In general, no measurement or test is perfect, and indeed, these imperfections affect our measurement results, in which case we obtain a measurement value and call the difference between the measured value and the presupposed value an error of a measurement. Thus, we conclude that the result of a measurement is always an "approximation" to the true value and is complete only when the measurement is accompanied by a statement of uncertainty of that "approximation". All components that affect the measurement uncertainty are evaluated with the "appropriate" methods and each method of calculating the measurement uncertainty is expressed as a "standard deviation" and is referred to as a "standard uncertainty" of a measurement.

These components of standard uncertainty combine to obtain the overall value of uncertainty known as "combined standard uncertainty". Like in everyday life, meeting the needs of industry, trade, health and safety, or other applications, "extended uncertainty" is usually required.
The aim is to provide a greater interval in relation to the result of a measurement than the standard uncertainty. All this is done in order to have a higher probability that within that extended uncertainty interval, we actually have the "true" value of the component we are measuring.
This is accomplished by multiplying the standard uncertainty with a safety factor "k". The choice of the safety factor is based on the probability of coverage or the level of security required[1].

2. ISO/IEC 17025:2017 requirements for measurement uncertainty

Testing laboratories as well as calibration laboratories when assessing measurement uncertainty, including all contributions that are significant and those arising from sampling, will be considered using appropriate measurements and tests. When the measurement or testing method excludes the rigorous assessment of measurement uncertainty, an assessment will be made on the basis of an understanding of the theoretical principles or practical experience of the method performance, the so-called Method A and Method B[2].
In cases where a measurement method or a well-known test determines the limits of the values of main sources of measurement uncertainty and specifies the form of presentation of the calculated results, as a requirement from the ISO/IEC 17025:2017 standard, it is considered that we have met point 7.6. 3 of this standard following the method of measurement or testing and reporting guidelines.
For a particular method where the measurement uncertainty is defined and verified, there is no need to estimate the measurement uncertainty for each result if we can show that the critical influencing factors identified are under control.
In assessing the uncertainty of measurement, we must take into account these factors:

- Requirements of applied methods
- Customer requirements
- Existence of acceptable limits for a certain measurement

In cases when we are dealing with the assessment of measurement uncertainty, we must also take into account important components such as: Etalons, reference materials, measurement methods, environmental conditions, calibration certificates, etc.
Measurement uncertainty is essential to the reliability of a measurement. Assessing measurement uncertainty is crucial when it comes to comparing different results, or assessing the relation to the limit values given by regulators. Sampling, pre-treatment, storage, transport from the place of sampling to the laboratory and tests are the main stages of the measurement process.
For the calculation of the measurement uncertainty, we use the methodology based on GUM[3] and Eurachem[4].

2.1. Specification of measurements

The process of selecting the parameters for determining the validity of the measurement, taking into account at least one parameter from each stakeholder they support, can be:

- Physic-chemical parameters;
- Solid content;
- Main ingredients;
- Nutrients;
- Organic matter and
- As appropriate.

[1] The Expression of Uncertainty in Testing, UKAS, Edition 3, November 2019
[2] Evaluation of the Uncertainty of Measurement in Calibration, EA-4/02 M: 2013
[3] Guidelines on the Determination of Uncertainty in Gravimetric Volume Calibration EURAMET Calibration Guide No. 19 Version 3.0 (09/2018)
[4] https://www.eurachem.org

2.2. Identify all sources (contributors) of uncertainty

In this paper we will describe the measurement of uncertainty with the empirical method which is based on duplication of samples and represent the advantage of including all sources of uncertainty without having to quantify them individually[5,6].

This methodology enables us to estimate the measurement uncertainty both for sampling and for measurements or tests in cases where they repeat. The analytical presupposition uncertainty is also assessed using laboratory data for the application of standard methods in the laboratory.

However, this methodology does not allow for a presupposed assessment of the samples. Participation in interlaboratory comparisons is necessary and would help us in the presupposed calculation of measurement uncertainty during sampling and these contributions could be estimated[7].

The main sources that contribute to the calculation of measurement uncertainty, that can be identified during sampling, handling, storage and transport may be:

- Heterogeneity of samples (time, space);
- Ordinary and extraordinary samples (sample volume, location);
- Sampling protocol (representative samples);
- Sampling equipment (protection from contamination);
- Environmental conditions (temperature and humidity);
- Sample handling (container type, bottle size, reagents added);
- Transport and storage (temperature and humidity, time);
- Sample stability for testing (testing delays);
- Other.

2.3. Calculation of measurement uncertainty

The measurement uncertainty (u^2) can be estimated empirically using the following equations, assuming that the measurement uncertainty (u) is described by the standard deviation:

$$u^2(\text{overall}) = u^2(\text{planned}) + u^2(\text{measured}) \tag{1}$$

With u^2 (overall), u^2 (planned), u^2 (measured), being respectively: the overall uncertainty, the uncertainty between the sampling target and the measurement uncertainty.

$$u^2(\text{measured}) = u^2(\text{sampling}) + u^2(\text{testing}) \tag{2}$$

With u^2 (measured), u^2 (sampling), u^2 (testing), being respectively: uncertainty during sampling and uncertainty of testing.

Extended uncertainty is calculated with the correction factor[8] k.

$$U = k*u \tag{3}$$

The final result of each measurement (Y) through the measurement uncertainty can be expressed:

$$Y = y \pm U \tag{4}$$

Or:

$$\text{Final result (Y)} = \text{Measured value (y)} \pm \text{Measurement uncertainty (U)}^9 \tag{5}$$

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[5] Measurement uncertainty arising from sampling. First Edition (2007) Editors: Ramsey MH (University of Sussex, UK) and Ellison SLR (LGC, UK)

[6] Grøn C, Bjerre Hansen J, Magnusson B, Nordbotten A, Krysell M, Jebjerg Andersen K, Lund U(2007) Uncertainty from sampling— a nordtest handbook for sampling planners on sampling quality assurance and uncertainty estimation.

[7] ISO 21748:2017, Guidance for the use of repeatability, reproducibility and trueness estimates in measurement uncertainty evaluation

[8] JCGM 100:2008, Guide to the expression of uncertainty in measurement

[9] Evaluation of the Uncertainty of Measurement in Calibration, EA-4/02 M: 2013

2.4. Calculation of Standard Deviation (S) and Z-score

The formula for calculating the standard deviation is:

$$S^2 = \frac{\sum(x_i - X_{mesatare})^2}{n-1} \tag{6}$$

Where:

S- Standard deviation
x_i - Number of samples taken
X - Average value
n – Number of samples (Minimum 5 measurements)

$$S^2 = \frac{(x_1 - X_{average})^2 + (x_2 - X_{average})^2 + (x_3 - X_{average})^2 + (x_4 - X_{average})^2 + (x_5 - X_{average})^2}{n-1}$$

The formula for calculating Z-score is:

$$Z = \frac{x_i - X_{average}}{S} \tag{7}$$

S- Standard deviation
x_i - Number of samples taken
X - Average value
n – Number of samples

The value of Z-score should be: $Z \leq 2$

Conclusion

Finally, we can say that the calculation of measurement uncertainty is crucial in ensuring that the measurements or tests are reliable and traceable. According to the many documents referred in this paper, as well as the ISO/IEC 17025:2017 standard, measurement uncertainty and metrological traceability are interdependent concepts. Furthermore, the process that includes the chain of measurements in calibration, testing laboratories and the process of product production, their marketing and assessment of uncertainties of those measurements or tests, is of great importance for both the metrologist and the laboratory or technologist who monitors the production process as that is an instrument for managing measurements. All this activity ultimately helps us to make decisions about where to invest in order to get better and more reliable results. On the other hand, international standards on measurement uncertainty provide a good basis for comparing measurement results between laboratories, and thus convince others and ourselves that our measurements and tests are reliable measurements and close to the values that we really expect. Carrying out as many measurements and tests, calculating the standard deviation, standard uncertainty, extended uncertainty and combined uncertainty, is done in order to have a higher probability within the uncertainty interval, ultimately knowing the value of what we measure.

Reference:

1. ISO/IEC 17025:2017, General requirements for the competence of testing and calibration laboratories
2. Evaluation of the Uncertainty of Measurement in Calibration, EA-4/02 M: 2013
3. The Expression of Uncertainty in Testing, UKAS, Edition 3, November 2019
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5. Measurement uncertainty arising from sampling. First Edition (2007) Editors: Ramsey MH (University of Sussex, UK) and Ellison SLR (LGC, UK)
6. Grøn C, Bjerre Hansen J, Magnusson B, Nordbotten A, Krysell M, Jebjerg Andersen K, Lund U (2007) Uncertainty from sampling— a nordtest handbook for sampling planners on sampling quality assurance and uncertainty estimation
7. ISO 5725-2:2019, Accuracy (trueness and precision) of measurement methods and results — Part 2: Basic method for the determination of repeatability and reproducibility of a standard measurement method
8. ISO 21748:2017, Guidance for the use of repeatability, reproducibility and trueness estimates in measurement uncertainty evaluation
9. JCGM 100:2008, Guide to the expression of uncertainty in measurement
10. https://www.bipm.org/en/home
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