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Guidelines for Uncertainty D#5.4

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2. Executive summary

This document constitutes Deliverable 5.4 of the JERICO project. It is intended to furnish members of the JERICO community with a basic understanding of uncertainty in measurement. The document presents the essential principles and concepts central to the determination of measurement uncertainty. It describes the different steps involved in an uncertainty calculation, and introduces reporting conventions. Some guidance on the proper preparation of relevant documentation is also included, and the importance of uncertainty determinations in the context of coastal marine observing activity is outlined.

3. Introduction

An uncertainty estimate is an integral part of a measurement result. No measured value can be considered complete without it. There are various reasons why uncertainty estimation is so vital in measuring activity, the main one being that it gives us a respectable measure of the ambiguity in the measurement result, and therefore some idea of the effective success of the measuring operation. Uncertainty estimates also tell us something about the trustworthiness of the data produced by the measuring activity, and are a key element in assessing their compliance against limits, whether normative or otherwise. Moreover, the correct estimation of the uncertainty is a key element for the assessment of results conformity.

Despite its importance, uncertainty is rarely discussed in marine observing circles, and is practically ignored in the marine data management community. The disregard is astonishing, given its obvious innate relation to performance, and data quality and usability issues.
Uncertainty is an intricate subject that is constantly evolving. The underlying concepts are complex, and based on rigorously precise definitions and terminology which need to be comprehended before they can be applied. The methodology is deceptively straightforward, and hard to apply in many real-life measuring circumstances, particularly when measurements are being made outside a controlled laboratory environment.

The generally accepted approach to evaluating and expressing uncertainties in measurements is given in the BIPM (Bureau International des Poids et Mesures) publication "Evaluation of measurement data - Guide to the expression of uncertainty in measurement", commonly referred to as the GUM (2008)[1]. The GUM presents a methodology for uncertainty estimations based on the propagation of the uncertainties associated with the individual variables involved in a measurement process, and provides recommendations and guidelines to assure conformity to first principles. However, it is a complicated treatise, and often needs to be supplemented with supportive simplifying documents to aid understanding and help in adapting the contents to specific fields of measurement.

This publication has been prepared to provide one such guidance document for members of the JERICO community. It presents the basic principles and main concepts underlying current practice in the determination and reporting of measurement uncertainty in a concise fashion. The different steps involved in an uncertainty calculation are explained briefly. Some

[1] This document can be downloaded as a PDF file or browsed online, complete with annotations, at the web address "http://www.bipm.org/en/publications/guides/gum.html".

Good Practice advice on proper documentation is given, and the utility of uncertainty determinations in the context of coastal marine observing activity is delineated.

The present document should not be employed as a substitute for the GUM. It is intended to be used *with* the GUM, which continues to remain the master reference document for the evaluation of uncertainty in measurement at this time.

4. Main Report

4.1. Some useful elementary concepts

An *observation* can be viewed as an item of information relating to a specific phenomenon, condition, aspect or feature of what is being studied obtained by direct scrutiny (i.e., using one or more of the five human senses without mediation of any kind) or indirect inspection (e.g. by means of specialized instrumentation).

A *property* is a distinctive attribute or feature that can be used to describe and/or characterize a system (or a process or a part of a system or process) or its state. Examples are the amount of substance, temperature, electrical conductivity, etc.

A *variable* is a factor, aspect or quantity which is subject to change.

Measurement is the process of experimentally obtaining one or more quantity values that can reasonably be attributed to a quantity; a quantity is a property of a phenomenon, body, or substance, where the property has a magnitude that can be expressed as a number and a reference.

A *measurand* is the quantity intended to be measured.

Data are the numerical results of a measuring process; "data" is a plural form (the singular form is "datum", although it is commonly used in the singular sense, also.

A comprehensive and endorsed vocabulary of metrological terms can be found in the document "International vocabulary of metrology - Basic and general concepts and associated terms (VIM) JCGM 200:2012[2].

4.2. Measurement and uncertainty

4.2.1 What is (and is not) a measurement?

As mentioned earlier, *measurement* is the process of experimentally obtaining one or more quantity values that can reasonably be attributed to a quantity; a quantity is a property of a phenomenon, body, or substance, where the property has a magnitude that can be expressed as a number and a reference. Measurement presupposes a description of the quantity commensurate with the intended use of a measurement result, a measurement

[2] This document can be downloaded as a PDF file or browsed online, complete with annotations, at the web address "http://www.bipm.org/fr/publications/guides/vim.html".

procedure, and a calibrated measuring system operating according to the specified measurement procedure, including the measurement conditions. A measurement result is the set of quantity values being attributed to a measurand, together with any other available relevant information. It is generally expressed as a single measured quantity value and a measurement uncertainty. The former consists of a number, denoting magnitude, that is a multiple of the unit of measurement - a real scalar quantity designated by conventionally assigned names and symbols, defined and adopted by convention, with which any other quantity of the same kind can be compared to express the ratio of the two quantities as a number. In practice, a measurement result is always obtained using some kind of instrument.

Scientific measurement always involves the implementation of a meaningful, quantifiable scale and a clearly defined system of units on that scale. The latter must be traceable, or at least relatable, to the International System of Units (SI). For these reasons, an arbitrary comparison such as that of two rods against each other to establish, for example, the length of one of them cannot be considered as measurements if a scale and unit system are missing.

4.2.2 What is measurement uncertainty?

The formal definition of the term "*uncertainty of measurement*" is as follows:

- parameter, associated with the result of a measurement, that characterizes the dispersion of the values that could reasonably be attributed to the measurand[3].

Another, more recent, definition is given below:

- non-negative parameter characterizing the dispersion of the quantity values being attributed to a measurand, based on the information used[4].

Simply put, the uncertainty of a measurement provides a quantitative estimate of the dubiousness of the measurement. This dubiousness arises because the "true" value of the measured property at the time of measuring is an idealized concept. Almost always, a measurement result can only approximate the true value owing to the many inherent imperfections and limitations of the measuring process, and the lack of exact knowledge of the measurand.

The uncertainty associated with a measurement is often reported as an *expanded uncertainty*, a quantity defining an interval about the result of a measurement that may be

[3] *Evaluation of measurement data - Guide to the expression of uncertainty in measurement*, Joint Committee for Guides in Metrology (JCGM) 100:2008.
[4] *International vocabulary of metrology - Basic and general concepts and associated terms (VIM)*, JCGM 200:2012.

expected to encompass a large fraction of the distribution of values that could reasonably be attributed to the measurand.

4.2.3 Error, accuracy and precision versus uncertainty

Error refers to the deviation of a measured value with respect to the true value. It is estimated and reported by subtracting the “true” value from the measured value, and can be positive or negative in sign. A measurement error is composed of two parts, one systematic (which is constant or varying in a predictable manner) and the other random (which changes unpredictably). The systematic component of the error can often be accounted for by applying an appropriate correction, although the resulting compensation may not always be perfect.

Note that uncertainty concerns the dispersion that could be reasonably expected of the result of a measurement about the true value (unknowable, by definition) under the specified measuring conditions. It should not be confused with the *accuracy* of a measurement, which is the closeness of agreement of the result to the best available estimate of the true value and is more closely related to the error of the measurement. It is possible for a measurement result to have a large uncertainty despite being very accurate, with a negligible error (Figure 1).

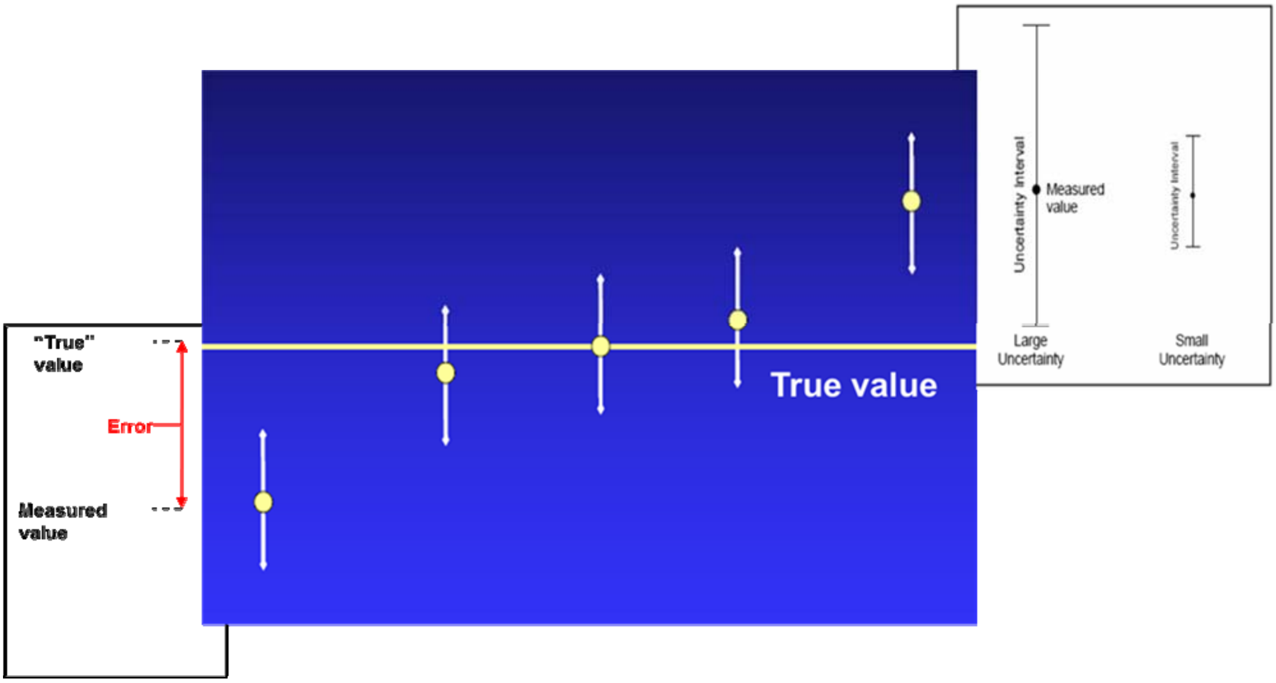


Figure 1. Error, accuracy and uncertainty.

Uncertainty also differs from the *precision*, described as the closeness of agreement between measured values obtained by replicate measurements under specified conditions, in that it is always associated with some characteristic probability distribution and an explicitly declared *level of confidence*.

4.2.4 Sources of uncertainty

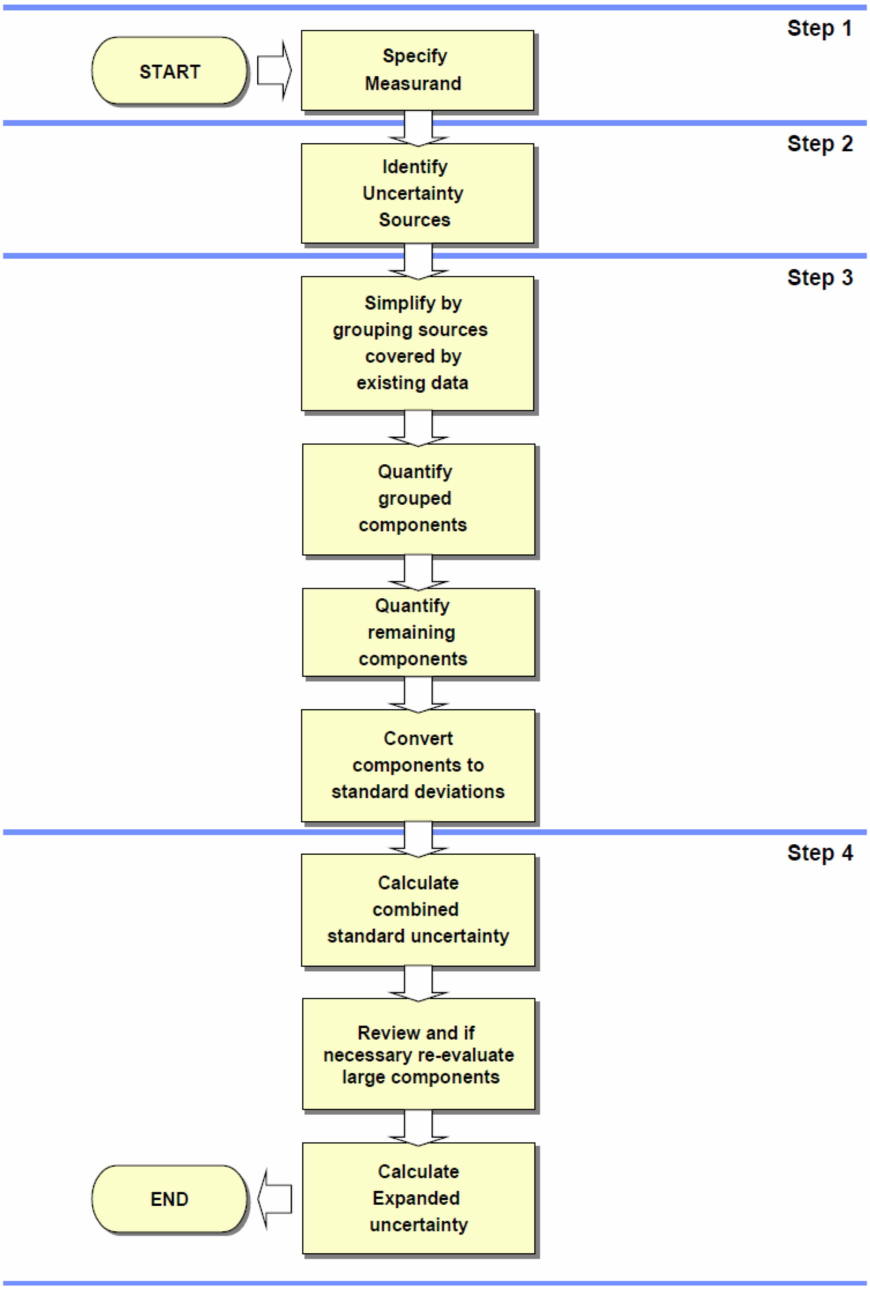
There are many possible sources of uncertainty in a measurement, and these sources need not necessarily be independent of each other. They include, and are not to be considered limited to, the following:

- weaknesses in the definition of the measurand;
- inexact realization of the definition of the measurand;
- non-representative sampling, i.e. the sample measured may not represent the defined measurand;
- influence of ambient effects on the measurement;
- finite instrument resolution or discrimination threshold;
- inexactness of measurement standards and reference materials;
- inexactness in the values of constants and other parameters obtained from external sources used in the measurement;
- approximations and assumptions incorporated in the measurement method and procedure;
- poor instrument precision.

4.3. Determining uncertainty

Typically, an uncertainty estimation involves the implementation of the following steps (Figure 2):

- the *definition* of the measurand;
- the *designation* of the sources of uncertainty relevant to the measurement;
- the *quantification* of the uncertainty components associated with these sources;
- the *calculation* of the total combined uncertainty of the measurement.



Source: *Quantifying uncertainty in Analytical Measurement*, EURACHEM/CITAC Guide CG4, Second Edition (2000).

Figure 2. The different steps in the uncertainty estimation process.

4.3.1 Defining the measurand

This is perhaps the most crucial and laborious step in the uncertainty evaluation process. Ideally, the step entails the unequivocal specification of what constitutes the measurand, in a way which provides unique values that describe it. Often, the realization of such values can implicate the use of special test material, measuring devices and setups, and particular environmental conditions. Take the case of practical salinity, for example. Here, the conductivity ratio (K_{15}) value of 1 corresponding to exactly 35 on the Practical Salinity Scale (PSS-78) is the defining point, but K_{15} itself is defined at the IPTS-68 temperature of 15 °C and the pressure of 1 standard atmosphere with respect to a potassium chloride (KCl) solution in which the KCl mass fraction is 0.0324356[5].

The definition of the measurand is also strongly governed by the accuracy requirements of the measurement. For example, a practical salinity measurement with an "electrode cell" type laboratory salinometer accurate to 0.002 (PSS-78) requires temperature to be held constant and accurate to within ±0.02 °C.

4.3.2 Designating the sources of uncertainty

This step is dependent on the previous one because the definition of the measurand will dictate, to a great extent, the number of elements and interactions of the measuring chain which will need to be taken into account while considering the sources of uncertainty in the measurement. Note that an outside factor that may only be influencing the measuring chain indirectly can also be a potential source of uncertainty in the measurement, and may need to be included in its overall uncertainty budget.

The general procedure for determining the sources of uncertainty in a measurement essentially comprises two tasks:

a) distinguishing their effects, usually done by means of a structured analysis using a *cause-and-effect* diagram (also known as an Ishikawa or 'fishbone' diagram).
b) reducing redundancy by dealing with duplicated contributions through *cancellation* (common effect, different times), *combination* (similar effect, same time) or *re-labelling* (similar effect, different times).

An example of a cause-and-effect diagram is shown in Figure 3.

[5] *Background papers and supporting data on the Practical Salinity Scale 1978*, Unesco technical papers in Marine Science 37, Unesco, 1981.

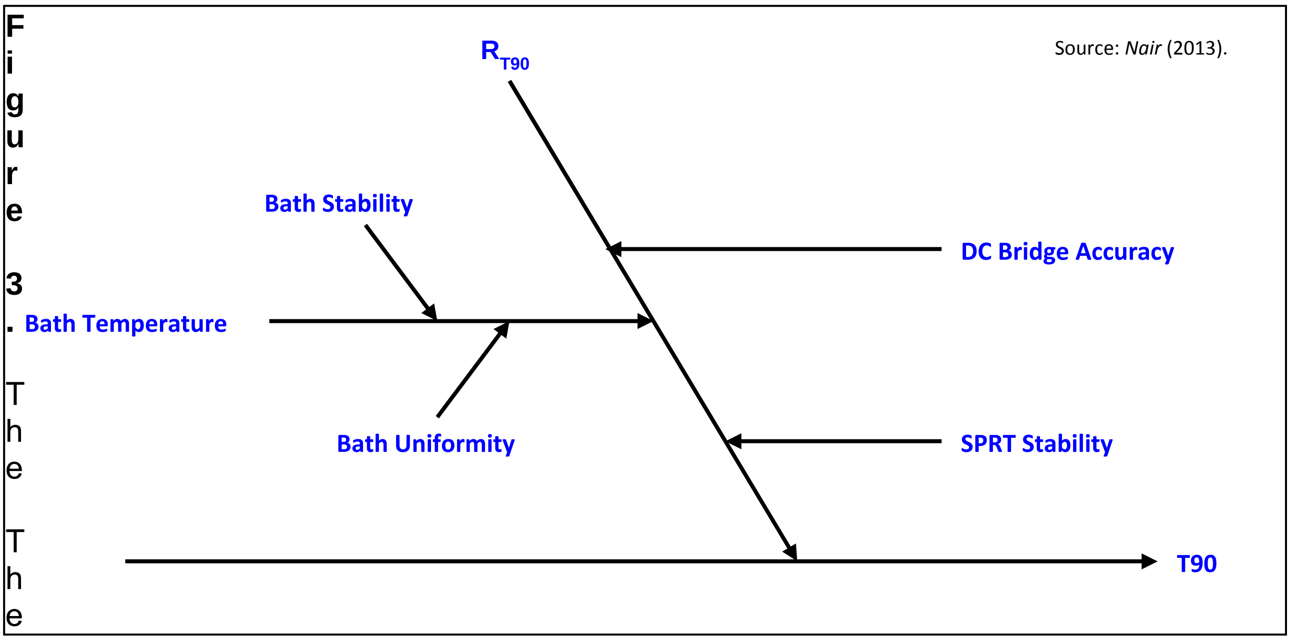


Figure 3. A simple cause-and-effect (Ishikawa) diagram for an ITS-90 temperature reading in a thermostatic seawater bath obtained from the measurement of the resistance (RT90) of an immersed Standard Platinum Resistance Thermometer (SPRT) made with a DC bridge apparatus; note that additional elements (e.g. bridge linearity, SPRT immersion error, etc.) can be included by adding new arrows appropriately.

4.3.3 Quantifying the uncertainty components

Once the different sources of uncertainty have been identified, their individual contributions to the total uncertainty of the measurement - in other words, the components of the uncertainty of the measurement - need to be quantified. This is done by estimating the *standard uncertainty* (*u*) expressed numerically as a *standard deviation*, associated with each source.

The evaluation of a standard uncertainty is classified as *Type A* or *Type B*, depending on the way it has been estimated. An evaluation is of Type A when the estimation is based on the statistical treatment of experimental data. In every other case, it is of Type B. For example, a value for the standard uncertainty extracted from an instrument manufacturer's specifications or from a calibration certificate would constitute a Type B evaluation.

A Type A evaluation is typically an estimate of the standard deviation obtained from real observations. A Type B evaluation, on the other hand, is usually an approximation of the

standard deviation, treated as being existent and adequately representative, based on the characteristics of a probability density function assumed to be sufficiently suitable for this purpose. Wherever appropriate, any covariances between different components should also be considered.

4.3.4 Calculating the combined uncertainty

This is the final step where the separate uncertainty components are summed up to calculate the *combined standard uncertainty* (u_c) of the measurement, according to the general relationship[6]:

$$u_c(y(x_1,x_2,\ldots)) = \sqrt{\sum_{i=1,n} c_i^2 u(x_i)^2} = \sqrt{\sum_{i=1,n} u(y,x_i)^2}$$

where $y(x_1,x_2,..)$ is a function of several parameters $x_1,x_2,...$, c_i is a *sensitivity coefficient* evaluated as $c_i = \partial y/\partial x_i$, the partial differential of y with respect to x_i, and $u(y, x_i)$ denotes the uncertainty in y arising from the uncertainty in x_i. When variables are not independent, the relationship is of the form:

$$u(y(x_{i,j\ldots})) = \sqrt{\sum_{i=1,n} c_i^2 u(x_i)^2 + 2\sum_{\substack{i,k=1,n \\ i\neq k}} c_i c_k \cdot u(x_i, x_k)}$$

where $u(x_i, x_k)$ is the covariance between x_i and x_k, and c_i and c_k are the sensitivity coefficients.

The sensitivity coefficients in the two formulations describe the dependencies of the value of y on the variability in the parameters x_1, x_2, etc. These coefficients may need to be evaluated experimentally, especially in the absence of mathematically definable relationships between parameters.

There are two methods that can be used to calculate the combined standard uncertainty:

a) the *analytical* method;

b) the *sequential perturbation* method.

In the analytical method, the computation is performed by applying one of the above two formulations, and requires the generation of partial differentials (or their numerical equivalents), making it unwieldy and impractical for complex measurement chains

[6] Quantifying uncertainty in analytical measurement, EURACHEM/CITAC Guide CG 4, Second Edition, QUAM: 2000.1.

involving many different parameters. The sequential perturbation method is based on the consequence of the Fundamental Theorem of Calculus, whereby it is possible to show that the uncertainty in the final measurement result can be estimated by sequentially perturbing the different parameters (x_1,x_2, etc.) appearing in the governing equations by their respective standard uncertainties. The relationship is of the form:

$$u_c = \sqrt{D_1^2 + D_2^2 + \cdots + D_i^2}$$

where

$$D_1 = y(x_1 + u_1, x_2, \ldots x_i) - y(x_1, x_2, \ldots, x_i),$$
$$D_2 = y(x_1, x_2 + u_2, \ldots x_i) - y(x_1, x_2, \ldots, x_i), \ldots$$
$$D_i = y(x_1, x_2, \cdots, x_i + u_i) - y(x_1, x_2, \ldots, x_i).$$

The method does not produce values as exact as those obtainable with the analytical approach, but it is easier to implement and allows for the evolution of the underlying measurement model.

4.3.5 Expanded uncertainty

In many commercial, industrial, and regulatory applications, particularly in the health and safety sectors, a measure of uncertainty must circumscribe an interval about the measurement result that may be expected to include a large fraction of the distribution of values that could reasonably be attributed to the measurand. The *expanded uncertainty* (*U*), obtained by multiplying the combined standard uncertainty by a *coverage factor* (*k*), provides just such a measure. The value of the coverage factor *k*, chosen on the basis of the *level of confidence* required of the interval, is usually 2 or, less often, 3.

4.4. Reporting uncertainty

4.4.1 The combined standard uncertainty (u_c)

When reporting the combined standard uncertainty u_c, its numerical value is stated alongside the value of the measurement result, usually in one of four ways. These ways are illustrated in the box shown in Figure 4 using the result of a weighing operation as an example.

Reporting expanded uncertainty U

“

Reporting combined standard uncertainty u_c

I

“m_S = 100.021 47 g with (a combined standard uncertainty) u_c = 0.35 mg.”

II

“m_S = 100.021 47(35) g, where the number in parentheses is the numerical value of (the combined standard uncertainty) u_c referred to the corresponding last digits of the quoted result.”

III

“m_S = 100.021 47(0.000 35) g, where the number in parentheses is the numerical value of (the combined standard uncertainty) u_c expressed in the unit of the quoted result.”

IV

“m_S = (100.021 47 ± 0.000 35) g, where the number following the symbol ± is the numerical value of (the combined standard uncertainty) u_c and not a confidence interval.”

Source: Evaluation of measurement data - Guide to the expression of uncertainty in measurement, Joint Committee for Guides in Metrology (JCGM) 100:2008.

Figure 4. The four recommended ways of reporting the combined standard uncertainty u_c associated with the measured value (m_S) of a nominally 100 g standard of mass.

4.4.2 The expanded uncertainty (U).

When reporting the expanded uncertainty *U*, its numerical value is stated alongside the value of the measurement result, as illustrated in the box shown in Figure 5 using the same information that was disclosed in Figure 4.

Figure 5. The recommended way of reporting the combined standard uncertainty *U* associated with the measured value (m_S) of a nominally 100 g standard of mass.

4.4.3 The uncertainty budget.

All the salient details concerning the determination of the uncertainty of measurement can be condensed and presented in tabular form as an *uncertainty budget*. Table 1 shows an example of such a budget, which in this case is related to the ITS-90 temperature measurement process described by the cause-and-effect diagram in Figure 3.

Temperature (ITS-90)				
Source	**Manufacturer's specification**	**Assumed probability distribution**	**Observed**	**Standard Uncertainty**
Temperature bath stability	0.002 °C	Triangular	---	0.0008 °C
Temperature bath uniformity	0.002 °C	Triangular	---	0.0008 °C
SPRT stability (at the Triple Point of Water)	---	---	0.0005 °C/year (2003 - 2010)	0.0005 °C
Precision Digital Thermometer accuracy	0.0015 °C	Rectangular	---	0.0009 °C
Combined standard uncertainty				0.0015 °C
Expanded Uncertainty (k = 2)				0.0030 °C

Source: Medeot, et. al., 2011.

Table 1. An example of an uncertainty budget, based on the cause-and-effect diagram for the ITS-90 temperature measurement process displayed in Figure 3 of this document.

Note that an uncertainty budget can be much more intricate than the one exhibited here. The level of detail will depend on the number of sources that need to be considered to achieve the final uncertainty estimate. The form of a budget and the way its different elements are computed can also vary.

4.4.4 Good Practice recommendations for preparing documentation.

Provide as much information as possible; the amount and degree of detail furnished must, at the very least, be sufficient enough to substantiate the fitness for purpose of the measurement results.

Record clearly all the methods and instrumentation used.

Outline the data analysis in a way that will permit easy repetition or re-evaluation, and independent corroboration of results, if necessary.

State all corrections and constants used in the analysis and their sources.

Take care to ensure that any information drawn from published material - such as, for example, an instrument calibration certificate - is up-to-date and relevant to the measurement process that was employed.

Avoid using an excessive number of digits while reporting numerical values.

Include an explicit exposition of the measurand, especially if there exist room for ambiguity regarding its definition.

4.5 Uncertainty evaluation in the context of coastal marine observatories

Establishing and reporting the uncertainty of measurement is mandatory in modern measuring practice for resulting data to be formally acceptable.

The uncertainty evaluation process subjects the whole measurement chain to critical scrutiny and analysis, leading to a clearer understanding of underlying operational mechanisms, better identification of shortcomings, and more efficient procedures.

Uncertainty estimates offer a sound basis for the design of realistic performance criteria for operating instrumentation.

Uncertainty estimates can assist in formulating judicious compliance criteria for measuring activities.

Uncertainty estimates are based on a universal methodology geared towards preserving internal consistency and transferability. This makes them perhaps the only truly reliable measure of the goodness of measurement results, and therefore indispensable for effective data quality assurance.

Uncertainty estimates provide valuable information for addressing usability issues, especially when dealing with pooled, multivariate, data coming from many sources, collected employing a variety of technologies on different spatial and temporal scales.

Data and data products incorporating uncertainty information tend to be more attractive and useful to users from mainstream productive sectors.

5. Conclusion

Measurement uncertainty is generally ignored, disregarded or overlooked in the marine observing and data management community, so much so that it is rarely declared, considered or even discussed. But, uncertainty is possibly the only concrete measure of how good data really are because it is intrinsically related to and consistent with the measuring processes that generate them.

Estimating uncertainty is a fundamental and necessary exercise in any kind of measuring activity. International norms recommend the incorporation of uncertainty information while reporting measurement results. Without this information, the value of the data produced is arguable, and the whole raison d'être of the measuring activity is open to question.

There is a pressing need to introduce and apply the concept of uncertainty in the marine observing field. The general theoretical and methodological framework for evaluating uncertainty in measurement already exists (in the GUM), but it will take incessant study, effort and innovative thinking to adapt it to the specificities of this singular sphere of activity.

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