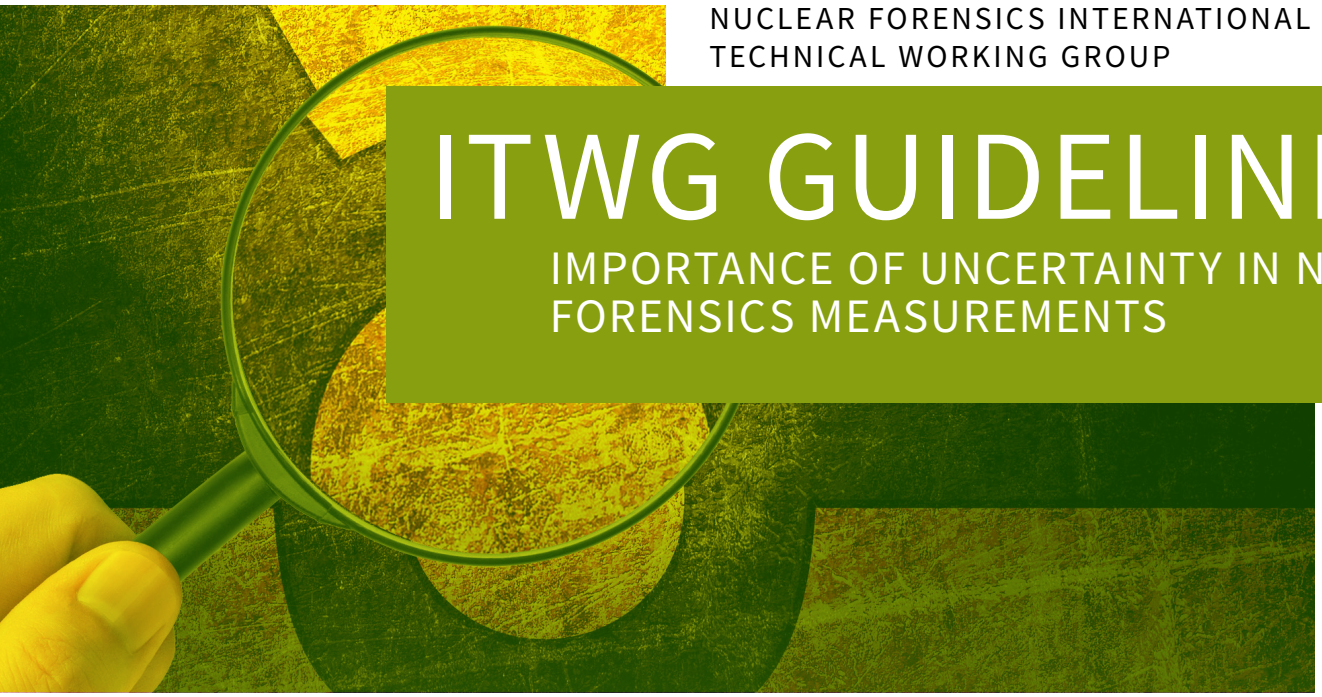
NUCLEAR FORENSICS INTERNATIONAL
TECHNICAL WORKING GROUP

ITWG GUIDELINE

IMPORTANCE OF UNCERTAINTY IN NUCLEAR FORENSICS MEASUREMENTS



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ITWG Guidelines are intended as consensus-driven best-practices documents. These documents are general rather than prescriptive, and they are not intended to replace any specific laboratory operating procedures.

1. WHAT IS MEASUREMENT UNCERTAINTY?

Uncertainty of measurement is the doubt that exists about the result of any measurement. An uncertainty is a quantitative estimate of the doubt associated with a measurement result. Although a measurement process attempts to determine the value of a chemical attribute or physical property, the actual measurement value is only an estimate of the true value. Measurement uncertainty characterizes the range of values within which the true value is asserted to lie, with a specified level of confidence. The International Organization for Standardization (ISO) defines measurement uncertainty as "A parameter associated with a result of a measurement, that characterises the dispersion of values that could reasonably be attributed to the measurand." Every measurement has an uncertainty associated with it, resulting from errors arising in the various stages of sampling, processing, and analysis and from imperfect knowledge of factors affecting the result. A measurement value has very limited basis of reliability without a statement of its uncertainty.

An uncertainty is therefore an assessment of the quality of a measurement. Uncertainty is the property of a specific value or measurement result. In contrast, bias and precision are properties of the measurement method that generated the result. Uncertainty should not be confused with error, which is the difference between the measured value and the true value. Uncertainty depends on the repeatability of the instrument, on the reproducibility of the result over time, on the number of measurements in the test result, and on all sources of random and systematic error that could contribute to a deviation from the true value. Contributions to uncertainty arise not only from the measurement procedure itself, but also from the repeated use of a reference material as a comparator or calibration standard and from the uncertainty of its certified value.

Why do we need Measurement Uncertainty?

- Integral part of Quality Assurance Systems for measurement results
- Required by accreditation regulations in many countries
- Required by ISO 17025
- Supports confidence and acceptance of measurement results
- Provides judgement on the significance of measurement differences
- Provides judgement on hypothesis and limit testing

The internationally accepted consensus method for estimating uncertainty is based on *The Guide to the Expression of Uncertainty in Measurement (GUM)*, published by ISO. It establishes general rules for evaluating and expressing uncertainty in measurements, is applicable to the wide range of methods employed in the nuclear and radiological community, and forms the basis for accreditation requirements relating to measurement uncertainty estimation. Consequently, GUM has been adopted by metrology institutes around the world and by a large number of nuclear and radiological laboratories.

2. WHY IS UNCERTAINTY IMPORTANT TO NUCLEAR FORENSICS?

The ability to accurately compare measurements, such as those used to characterize a series of nuclear material seizures by law enforcement, requires an associated statement of uncertainty. An uncertainty statement is particularly important when comparing measurement results among different nuclear laboratories or among different techniques. An assessment of different results can only be made on the basis of two values agreeing (or not agreeing) within the uncertainty of their measurements. Meaningful interpretation is nearly impossible without an assessment of uncertainty.

As an illustration of the use of uncertainties, in Figure 1 two graphs with identical measurement values are shown, one with and the other without uncertainties displayed as vertical bars. Each measurement result (diamond symbols) represents a separate interdiction, seizure, and analysis of HEU in a separate country. Security officials among the three nations are cooperating and want to know if the three materials are the same, and thus potentially link events, sources, routes, etc., for the purpose of attribution. Without the use of uncertainties, the only valid conclusion from the measurement data alone is that the interdictions are not related. Taking measurement uncertainty into consideration, the interpretation of the data plotted in the right diagram leads to the assessment that given the overlapping uncertainties of Nation X and Nation Y, two of the interdictions are related with regard to U-235 abundance. Security officials could then compare and corroborate this conclusion with other evidence.

The admissibility of nuclear forensics measurements in a court of law, and opinions derived from these data, is strongly dependent on the validity of the data. Courts have ruled that data must result from validated scientific methods whose principles and application can be justified. The use of uncertainties when reporting results is a key requirement to justify valid data, and in conjunction with the use of certified reference materials, fulfills the need for traceability to national or international reference standards. Traceability provides a means to relate measurements performed at different times by different analysts and by different methods to a

consistent measurement base or scale. The analyst must also ensure that nuclear forensic analytical methods are validated by using repeatable measurements with comparison to appropriate standards, permitting determination of detection limits and related parameters that influence uncertainty. Validation is an important process tool used to justify confidence in a technique and a necessary requirement for laboratory accreditation. Forensic laboratories in several countries have developed elaborate quality assurance systems and quality control procedures to ensure that their analyses meet the current standards of legal scrutiny and to ensure that scientific data and opinion is acceptable in criminal and civil court proceedings.

An accurate statement of confidence for the results of a nuclear forensic investigation is vital when communicating results to senior government officials and decision makers. An incorrect conclusion derived, for example, from an over-confident assessment of technical nuclear forensic data could mis-identify the source or origin of a material that may lead to inappropriate national or international actions with adverse consequences. An uncertainty provides confidence in the value of the measurement, judgment on significance of differences between measurement results, information regarding the capability of the measurement procedure, and quality assurance.

Why is GUM Uncertainty Important to Nuclear Forensics?

- Allows justifiable comparison of measurement results from different material seizures
- Allows justifiable comparison of measurement data with national nuclear library information
- Allows traceability of measurements to national and international standards and reference bases
- Improves admissibility of results in a court of law
- Internationally credited/accepted approach to calculating and expressing uncertainties
- Allows everyone to 'speak the same language'
- Allows the term 'uncertainty' to be interpreted in a consistent manner
- Increasing use by the nuclear forensics community

3. ESTIMATING UNCERTAINTIES USING 'GUM'

An analyst seeking to establish uncertainty estimates for technical nuclear forensics methods needs to develop a strategy for propagating uncertainty that integrates multiple sources and types of information. The GUM stresses that uncertainties should be evaluated by compiling and adding individual uncertainty components, whether arising from systematic or random effects. The GUM differs from previous error analysis in its use of a measurement equation for each analytical procedure. This is used to propagate standard uncertainties and correlation coefficients of the various input quantities. This mathematical equation describes the functional relationship between the measured value and the influence quantities (those input parameters that influence the measured result), and is relatively easy to create. Uncertainty components (standard deviations) and associated sensitivity coefficients are combined by quadrature (square root-sum-of-squares, Figure 2) and evaluated as an expanded uncertainty to provide coverage with a high level of confidence. Sensitivity coefficients (c_i) are partial derivatives of the model equation with respect to the input quantities (x_i), where $c_i = \partial_f/\partial x_i$.

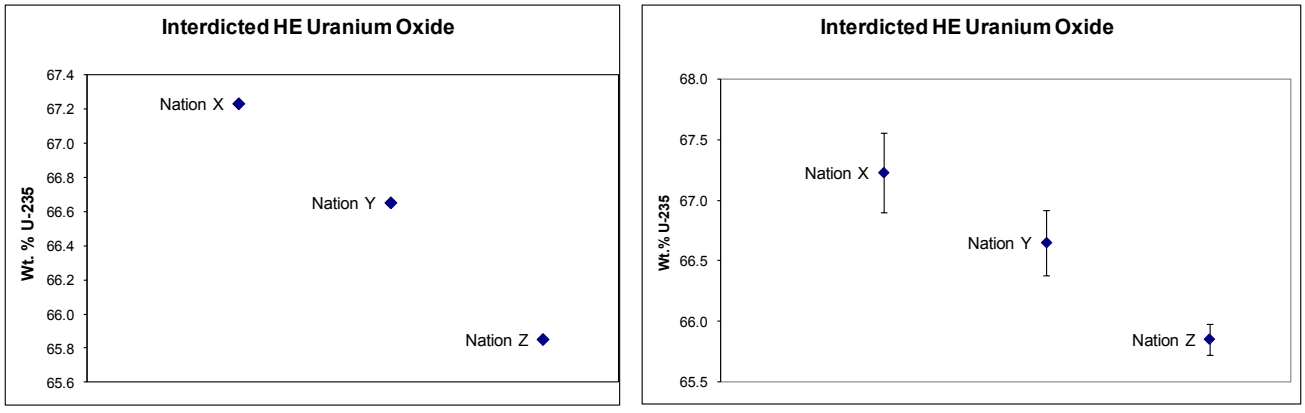

Fig. 1. Hypothetical examples of U-235 data, reported with (right) and without (left) uncertainties.

Fig. 2. Basic formula for combining uncertainty

$$u_c(y) = \sqrt{\sum_{i=1}^{n} [c_i * u(x_i)]^2}$$

where:

$u_c(y)$ = combined standard uncertainty

c_i = sensitivity coefficient

$u(x_i)$ = standard uncertainty

GUM incorporates the uncertainty associated with reference standards and fundamental constants in a consistent way. It also accounts for the uncertainty associated with the correction of systematic effects. Although GUM provides a more unified structure for uncertainty propagation, the analyst is given considerable freedom under GUM to use non-statistical methods to quantify components of uncertainty (so called Type B evaluation).

A GUM calculation requires statistical information on measurement imprecision and the correction for systematic effects. The analyst can generally approach a GUM calculation in one of two ways. The first approach is where the highest confidence levels are required, where the analyst attempts to quantitatively isolate and evaluate all significant components or sources of error, often through separate tests, which can be a very involved process. Alternatively, with use of properly matched reference materials (and corroborated by validation tests), it is possible to subsume the necessary uncertainty components through repeated measurement of reference materials and the unknown sample. In either case, the assessment of systematic uncertainty, in general, must be made by comparison to a standard, but it may be estimated using experiments designed for that purpose, or from verification of two or more independent and reliable methods, often termed orthogonal verification. Both approaches are amenable to the use of commercial software.

In brief, the steps for calculating the expanded uncertainty of any value are:

Step 1: Specify the measurand

Step 2: Identify the uncertainty sources

Step 3: Calculate the standard deviations

- Simplify by grouping sources covered by existing data
- Quantify grouped components
- Quantify remaining components
- Convert components to standard deviations

Step 4: Calculate expanded uncertainty

- Calculate combined standard uncertainty
- Review and, if necessary, re-evaluate large components
- Calculate expanded uncertainty

The merits of GUM are the transparency of the uncertainty evaluation, the treatment of uncertainties in a consistent logical way, and the presentation of an uncertainty budget resulting in a feedback to the analyst (i.e., identifies the dominant components of uncertainty and allows better understanding and improvement of the measurement process). An important advantage of GUM is that it provides a common framework to compare measurement results from different laboratories or different analytical methods. Because uncertainties that follow GUM principles are in general transparent and comparable, an assessment of different results can be made on the basis of the two values agreeing within the uncertainty of their measurements.

4. WHAT EFFORT IS NEEDED TO IMPLEMENT UNCERTAINTY ESTIMATION?

The quality and usefulness of an uncertainty estimate is dependent on the operator's detailed knowledge of the measurement process and the ability to properly evaluate the magnitude of the uncertainty components. As noted, uncertainty may be evaluated by quantifying and combining individual sources of uncertainty, or estimated, for example, from measurement data of certified reference materials obtained from a method validation study.

The calculation of GUM uncertainties follows a prescribed process and requires a commitment of time and human resources to implement for the first time. A GUM calculation procedure for a facility-specific analytical method can typically be designed and implemented by experienced chemists or analysts (as opposed to experienced GUM practitioners) within several weeks. The interested reader is directed to the Eurachem/CITAC guide, Quantifying Uncertainty in Analytical Measurement, which can be obtained for free at http://www.measurementuncertainty.org. This is an excellent tutorial with several example calculations derived from

analytical chemistry. Uncertainty calculations can be implemented in an Excel™ spreadsheet, or through the use of commercial software designed for various measurement and testing fields (e.g., GUM Workbench™).

5. DEFINITIONS OF RELEVANCE TO UNCERTAINTY AND MEASUREMENTS

The following selected terms are commonly used in association with the estimation of uncertainty, and are provided to show their current use and meaning. Their inclusion here is meant to help clarify the current concepts. Definitions are quoted from the BIPM Vocabulary in Metrology, Eurachem/CITAC guides, and Taylor and Kuyatt (see References).

Accuracy: the closeness of agreement between a test result and the accepted reference value. Accuracy consists of two components, namely trueness and precision; precision includes repeatability and reproducibility. It is noted that the common expression of accuracy is 'measurement uncertainty,' which provides a single value in expressing accuracy.

Bias: the difference between the expectation of the test results and an accepted reference value.

Combined Standard Uncertainty (u_c): standard uncertainty of the result of a measurement when the result is obtained from the values of a number of other quantities equal to the positive square root of a sum of terms, the terms being the variances or co-variances of these other quantities weighted according to how the measurement result varies with these quantities.

Coverage Factor (k): numerical factor used as a multiplier of the combined standard uncertainty in order to obtain an expanded uncertainty. Note that a coverage factor is typically in the range or 2 to 3.

Expanded Uncertainty (U): the quantity defining an interval about the result of a measurement that may be expected to encompass a large fraction of the distribution of values that could reasonably be attributed to the measurand. Note that an expanded uncertainty U is calculated from a combined standard uncertainty u_c and a coverage factor k using: $U = k \bullet u_c$.

Measurand: quantity intended to be measured.

Precision: the closeness of agreement between independent test results obtained under stipulated conditions.

Random Error: result of a measurement minus the mean that would result from an infinite number of measurements of the same measurand carried out under repeatability conditions. In a measurement uncertainty evaluation, this roughly corresponds to "component of uncertainty arising from a random effect".

Repeatability: closeness of the agreement between the results of successive measurements of the same measurand carried out under the same conditions of measurement.

Sensitivity Coefficient: The sensitivity coefficient shows the relationship of the individual uncertainty component to the standard deviation of the reported value for a test item. Mathematically, sensitivity coefficients are partial derivatives of the model function with respect to the input quantities. Sensitivity coefficients are effectively the GUM term for conversion factors that convert from input quantity units into units of the measurand.

Standard Uncertainty: uncertainty of the result of a measurement expressed as a standard deviation.

Systematic Error: difference between the mean that would result from an infinite number of measurements of the same measurand carried out under repeatability conditions and a true value of the measurand. In a measurement uncertainty evaluation, this roughly corresponds to "component of uncertainty arising from a systematic effect".

Trueness: the closeness of agreement between the average value obtained from a large series of test results and an accepted reference value. Trueness of a method is typically expressed in terms of its opposite, the method bias.

Uncertainty: a parameter associated with the result of a measurement that characterizes the dispersion of the values that could reasonably be attributed to the measurand. See also Expanded Uncertainty, Standard Uncertainty, Combined Standard Uncertainty.

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