National Analytical Management Program (NAMP)
U.S. Department of Energy Carlsbad Field Office

Radiochemistry Webinars

Environmental/Bioassay Radiochemistry Series

Guide to the Expression of Uncertainty (GUM)

In Cooperation with our University Partners

Meet the Presenter…

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Mr. Soriano worked at the International Atomic Energy Agency's Safeguards Analytical Laboratories (SAL) located in Seibersdorf, Austria, upgrading their LIMS. He has served as an adjunct professor at the former DOE Central Training Academy, working in course development and presentation of various statistical topics in nuclear safeguards. Mr. Soriano received his M.S. in Statistics from the University of Illinois in 1979, and his B.A. in Mathematics from Colorado College in 1977. He is a member of ASTM Committee C26 on the Nuclear Fuel Cycle and previously served as the head of Subcommittee C26.08 on Quality Assurance, Statistical Applications, and Reference Materials.

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NEW BRUNSWICK LABORATORY

Understanding the Guide to the Expression of Uncertainty (GUM)

Michael Soriano

NEW BRUNSWICK LABORATORY

Target audience

- Project planners
  - who should understand the proper role of measurement uncertainty in planning
- Data users
  - who need to understand the impact of measurement uncertainty in decision-making
- Data producers (e.g., chemists and count room personnel)
  - who should understand the significance of uncertainty in their measurement results

Outline

- Fundamental concepts of measurement uncertainty
  - Introduction to GUM concepts and terminology
  - Methodology of GUM evaluation
- Software approaches and tools to perform a GUM evaluation
  - Analytical approach
  - Numerical approach
    - Kragten Spreadsheet
    - GUM Workbench
  - Monte Carlo approach
- Interpretation of GUM evaluation
  - What does the expanded uncertainty mean?
  - The uncertainty budget
- Example of GUM evaluation

Definition of Uncertainty

Uncertainty of measurement:

- Parameter, associated with the result of a measurement, that characterizes the dispersion of the values that could reasonably be attributed to the measurand (GUM and VIM)

Uncertainty Concepts

- All measurements are subject to random and systematic measurement errors
- Uncertainty evaluation indicates how well a measured value may reflect the associated true quantity in a quantitative manner
- Quantification of uncertainty is basis for comparisons between measured values or methods
- Traceability of measurements requires quantification of uncertainty

Value of GUM

GUM is needed and will improve, for example:

- Research and development, engineering
- Enforcing laws and regulations
- Trade
- International comparison of measurement standards
- Calibration, quality assurance, accreditation, and certification
- Generating reference data
- Judgment of safety risks

GUM Concepts

Just as the use of the International System of Units (SI) brings coherence to measurements …

…the International Organization for Standardization (ISO) Guide to the Expression of Uncertainty in Measurement (GUM) represents a standardized way of expressing uncertainty in measurements

GUM History

The ISO GUM Guide was developed by seven international scientific organizations:

- International Bureau of Weights and Measures (BIPM)
- International Electro-technical Commission
- International Federation of Clinical Chemistry
- International Organization for Standardization (ISO)
- International Union of Pure and Applied Chemistry (IUPAC)
- International Union of Pure and Applied Physics
- International Organization of Legal Metrology

GUM History (cont.)

- The first edition of *The Guide to the Expression of Uncertainty in Measurement* (GUM) was issued by ISO on behalf of the member organizations in 1993. It has been revised several times since the first edition.
- Most recently, a new international organization, the Joint Committee for Guides in Metrology (JCGM), was formed to assume responsibility for the maintenance and revision of the GUM. The JCGM is composed of the seven international organizations listed previously, with the addition of the International Laboratory Accreditation Cooperation (ILAC).

GUM Terminology

- A quantity subject to measurement (called **measurand**) is stated with its **value**, **uncertainty**, and **unit**

- For example, m = (10.0 ± 0.1) g
- Where
  - m (a mass) is the **measurand**
  - 10.0 is the **value** of the measurand
  - 0.1 is the **uncertainty** of the measurand
  - g (grams) is the **unit** of the measurand

Gum Components

The components of an uncertainty evaluation include:

- A measurement equation
- A statistical model of each input to the measurement equation
- Data or other information about each input
- Estimates of the unknown parameters in the models of each measurement process component based on the data
- Statistical (Type A) methods for parameter estimation
- Non-statistical (Type B) methods for parameter estimation
- Mathematical procedures for combining the uncertainties from each part of the measurement process in an appropriate manner

Measurement Equation

- A measurement equation is a mathematical formula or function that shows how all the necessary quantities are combined to obtain a desired measurement result
- The quantities used in measurement equations are typically summary statistics obtained from statistical models of the process components
- Most quantities in a measurement equation will have uncertainties that contribute to the total uncertainty of the measurand; however, some theoretical quantities may not contribute any uncertainty to the final result

Mathematical Model of the Equation

In a mathematical format:

- $M = f(x_1, x_2, \ldots, x_n)$ where M is the measurand, f is the measurement function, and the x_is are the inputs to the measurement function
- Each x_i has a value, a statistical model or distribution associated with the value and a corresponding standard uncertainty symbolized by $U(x_i)$

Measurement Equation Example 1

- The simplest possible measurement equation is

$$Y = f\left(X_1\right) = X_1$$

where: Y is a final measurement result, and

X_1 is a summary of direct replicate measurements of the measurand

Measurement Equation Example 2

- A more complicated measurement equation might look like

$$Y = f\left(X_1, X_2, X_3, X_4\right)$$

$$= \frac{X_1 - X_2}{X_3} + 2X_4$$

where: Y is a final measurement result, and

X_1- X_4 are summaries of different input quantities

Properties of a Good Measurement Equation

A good measurement equation (ME) should:

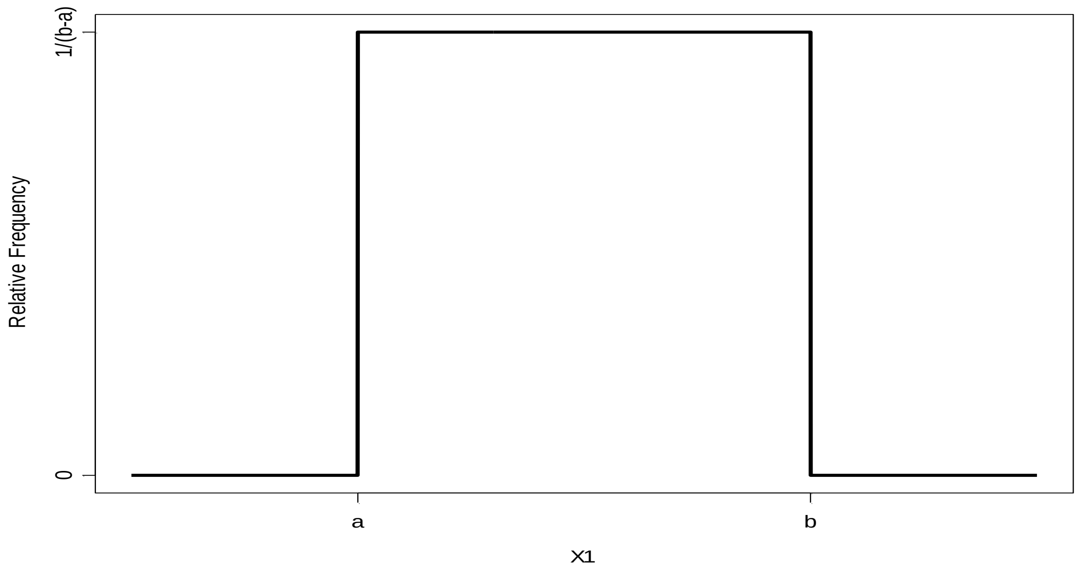
- Provide an adequate approximation to the value of the quantity of interest
- Include an input value for every source of uncertainty

Measurement Equation Inputs

- To understand the total uncertainty in a measurement result, we first study or model each input to the measurement equation individually to understand its uncertainty
- Statistical models are used to describe each component of the measurement process in terms of the possible values it can produce
- Probability distributions are used in these models to quantitatively describe the relative frequencies of occurrence of the values each input to the measurement equation can take on

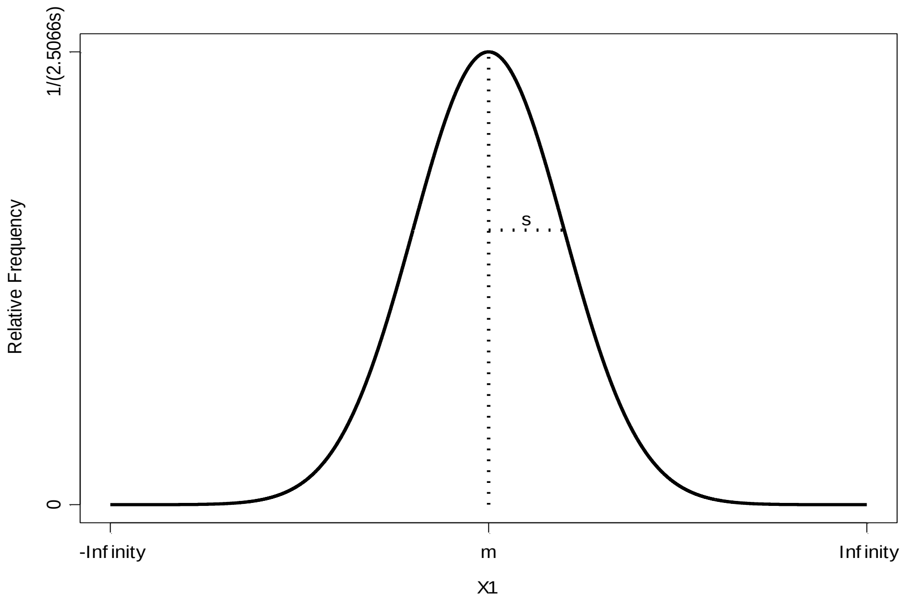
Probability Distribution Example 1

- A uniform distribution would be a good description of a measurement process component whose values are equally likely to be anywhere between a lower and upper bound



Probability Distribution Example 2

- A normal distribution would be a good description of a measurement process whose values are centralized and are unbounded



Probability Distribution Parameters

- While the probability distributions just shown give a good picture of the relative frequencies with which different measurement results might occur, they are still too complicated for convenient use
- The locations of the distribution’s end points or the distribution’s central value and average width can be used as simpler representations of each distribution
- These numbers that concisely describe the location and scale of a probability distribution are called the **parameters** of the distribution

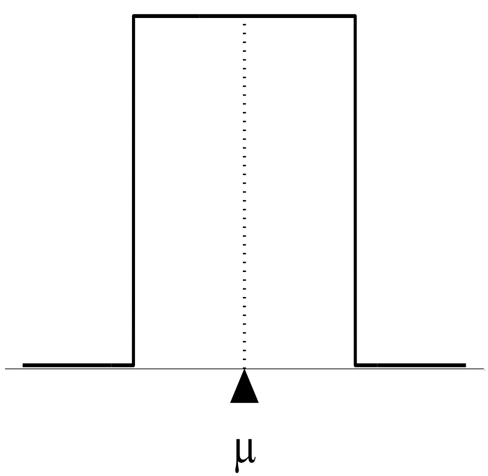
Probability Distribution Parameters

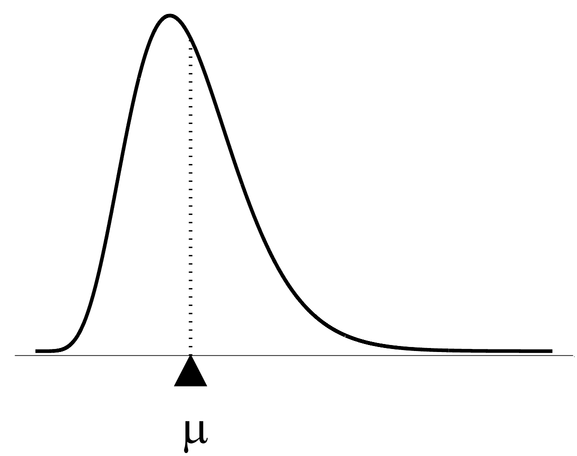
- As shown in the examples, the uniform distribution can be naturally parameterized by its end points
- The normal distribution has no end points, however, and is instead characterized by its central value and average width
- For consistency, we will use the central values and average widths to describe other distributions also
- Using the central values and average widths to summarize each distribution will provide a manageable amount of information and will be convenient for later calculations

Probability Distribution Mean

- The central value of each distribution is called **the mean of the distribution** and will be denoted by the symbol μ

- μ is the center of gravity for the distribution





Probability Distribution Standard Deviation

- The average width of each distribution is called the **standard deviation** of the distribution and will be denoted by the symbol σ
- σ gives the typical absolute deviation between a random observation from the distribution and μ

Sampling from the Measurement Process

- Since the probability distribution used to describe the measurement process actually describes the infinite number of potential results from the measurement process, we can never directly observe μ or σ

- Instead, a limited amount of data from the process serves as a representative sample of the measurement process and is used to estimate the unknown parameters

- The "data" used to estimate the unknown parameters of the distribution can be either statistical data or some type of non-statistical information

Parameter Estimation: Type A

- Statistical data are obtained by taking a random sample of measurements made under identical conditions from the measurement process
- When statistical data are available, appropriate summaries of the data are used to estimate the values of the unknown parameters from the probability distribution that describes the measurement process
- Measurement equation components whose parameters have been estimated using statistical methods are classified as **Type A components**

Statistical (Type A) Methods for Estimating μ

- The most popular estimator for μ is the **sample mean**:

$$\bar{X} = \frac{1}{n}\sum_{i=1}^{n} X_i$$

- $\bar{X}$ makes a good estimator for μ because the observed values larger than μ tend to offset values smaller than μ when the X_i are summed, making $\sum X_i \sim n\mu$

Statistical (Type A) Methods for Estimating σ

- Analogous to the sample mean, the most popular estimator for σ is the sample standard deviation:

$$S = \sqrt{\frac{\sum_{i=1}^{n} (X_i - \bar{X})^2}{n-1}}$$

- Because we know $\bar{X} \approx \mu$, each $(X_i - \bar{X})^2$ should be near $(X_i - \mu)^2$; the theoretical values that σ is based on. Averaging these values tends to even out any errors and makes *S* a good estimator for σ

Estimating the Standard Deviation of the Mean

- Although S is a good estimate of the variation in X_i, it does not tell us how to estimate the standard deviation of $\bar{X}$, the quantity we will use to estimate μ
- Based on the propagation of uncertainty for linear measurement equations, it can be shown that the standard deviation of $\bar{X}$ is $\sigma/\sqrt{n}$
- Therefore, if S is a good estimate of σ, then $S/\sqrt{n}$ will be a good estimate of $\sigma/\sqrt{n}$
- In the ISO Guide, $S/\sqrt{n}$ is called the **standard uncertainty** of $\bar{X}$ and is denoted $u(\bar{X})$

Use of S Versus $S/\sqrt{n}$ in Uncertainty Analysis

- Use of S, rather than $S/\sqrt{n}$, as the standard uncertainty of a mean, $\bar{X}$, is a very common mistake in uncertainty analysis
- It is likely you will see other people do this, but you should not make the same mistake
- The correct standard uncertainty for a mean in most situations is going to be $S/\sqrt{n}$

Expanded Uncertainty Versus Standard Uncertainty

- After estimating the combined standard uncertainty of a measurement result, u_c, the final task to complete the uncertainty analysis is to compute its **expanded uncertainty**, which is denoted U

- The expanded uncertainty is computed using the formula:

$$U = ku_c(Y)$$

- The **coverage factor**, typically denoted k, controls the probability with which the measurement result ± its expanded uncertainty will contain the measurand

- For large samples, a coverage factor of k = 2 is used when a coverage probability of 95% is desired

Expanded Uncertainty Versus Standard Uncertainty

- A combined standard uncertainty quantifies how much a measurement result will typically deviate from the measurand
- An expanded uncertainty quantifies how much a measurement result will deviate from the measurand with a high probability, often approximately 95% or 99%
- Expanded uncertainties are often reported because people want to know something about all plausible values the measurand may have
- Ideally, an expanded uncertainty interval will have an explicitly stated probability level that quantifies the probability with which the measurand lies in the interval

Parameter Estimation: Type B

- Non-statistical types of information that can be used to estimate the unknown distributional parameters include:
  - Scientific judgment
  - Manufacturers' specifications
  - Other indirectly related or incompletely specified information
  - Stated uncertainties on a certified value of a Certified Reference Material (CRM)

- Measurement equation components whose parameters have been estimated non-statistically are classified as **Type B components**

Rationale for Type B Uncertainties

- Type B uncertainties are needed because statistical data that reflect the natural variation in a measurement value from a particular source are not always available when a measurement result is needed

- Data on a Type B source of uncertainty may not be available because
  - The variation in the measurements from that source of error changes much more slowly than other sources of error
  - The particular factor in question was not known to affect the measurement process until after the measurements were made
  - The cost of collecting statistical data may be too high

- Uncertainty sources that must be assessed using Type B methods do affect the process, however, and must be accounted for in the final measurement results

Keeping Type B Uncertainty Methods in Perspective

- Due to the typical uses of Type B uncertainties and the techniques used to obtain them, it can be easy to lose sight of the nature of uncertainties assessed using Type B methods
- Type B uncertainties are essentially based on scientific judgment and are therefore subjective and personal
- The special methods for obtaining Type B uncertainties are designed to help ensure that scientists with a shared point of view reach the same conclusions when analyzing data and to make comparison of subjective uncertainties easier

Uncertainty of Linear Measurement Functions

- Measurement equations of the form $Y = c_i \bar{X}_i + c_j \bar{X}_j + \ldots + c_0$ in which all of the coefficients, c_i, c_j, and c_0 are constants, are linear measurement functions

- For this subset of measurement functions, when $\bar{X}_i$ and $\bar{X}_j$ are estimated independently of one another, we know from statistical theory that the **combined standard uncertainty** of *Y* is given by

$$u_c(Y) = u_c\left(f\left(\bar{X}_i, \bar{X}_j\right)\right) = \sqrt{c_i^2 u_i^2 + c_j^2 u_j^2 + \ldots}$$

where u_i and u_j are the standard uncertainties of $\bar{X}_i$ and $\bar{X}_j$

Linearization of Nonlinear Measurement Equations

- Knowing how to compute uncertainties for linear measurement equations, we can approximate the uncertainty for nonlinear measurement equations if they can be linearized
- From calculus, we know that any differentiable function can be well approximated by a linear function in a small region
- Taylor series can be used to find out what line makes a good approximation for the measurement equation near the value of the measurand

Linearization of Nonlinear Measurement Equations (cont.)

- The first order Taylor series for values of the function $f(\bar{X}_1, \bar{X}_2, \ldots)$ near $f(\mu_1, \mu_2, \ldots)$ is given by

$$f(\bar{X}_1, \bar{X}_2, \ldots) \approx f(\mu_1, \mu_2, \ldots) + \left[\frac{\partial f}{\partial \bar{X}_1}\right](\bar{X}_1 - \mu_1) + \left[\frac{\partial f}{\partial \bar{X}_2}\right](\bar{X}_2 - \mu_2) + \ldots$$

  where $\left[\frac{\partial f}{\partial \bar{X}_i}\right]$ is the partial derivative of the measurement equation with respect to the i^{th} input to the measurement equation evaluated at $\bar{X}_i$

- Partial derivatives quantify how much the value of a multivariable function changes when one specific input is changed by 1 unit

Propagation of Uncertainties for Linearized Measurement Equations

- Treating the partial derivatives as constants and applying the rules we know for the uncertainty of linear measurement equations with independently estimated inputs gives an approximate combined uncertainty of

$$u_c\left(Y\right)=u_c\left(f\left(\bar{X}_1,\bar{X}_2,\ldots\right)\right)\approx\sqrt{\left[\frac{\partial f}{\partial\bar{X}_1}\right]^2u_{\bar{X}_1}^2+\left[\frac{\partial f}{\partial\bar{X}_2}\right]^2u_{\bar{X}_2}^2+\ldots}$$

Note: Treating the partial derivatives as constants is consistent with the use of the linear approximation

Propagation of Uncertainties for Linearized Measurement Equations

- The partial derivatives that scale each standard uncertainty to obtain the combined uncertainty are called **sensitivity coefficients**
- To lessen the burden of the notation when writing out results, the sensitivity coefficients are typically denoted by $c_{\bar{X}_i}$ rather than the notation $\partial f / \partial \bar{X}_i$

(Output Variation)=(Sensitivity)*(Input Variation)

- As illustrated in the formula for $u_c(Y)$, uncertainty in Y arises from both sensitivity and random variation

$$u_c(Y) = u_c\left(f\left(\bar{X}_1, \bar{X}_2, \ldots\right)\right) \approx \sqrt{c_{\bar{X}_1}^2 u_{\bar{X}_1}^2 + c_{\bar{X}_2}^2 u_{\bar{X}_2}^2 + \ldots}$$

- Sensitivity coefficients indicate the rate at which variation in the input is converted to corresponding variation in the output for a particular function

- Standard uncertainties for the inputs indicate how much input variation there is to be converted

Avoiding Hidden Correlations

- "Bad" ME, which hides correlation between Y_1 and Y_2

$$Y = \frac{Y_1}{Y_2}$$

$$Y_1 = \bar{X}_1 + \bar{X}_2 \qquad Y_2 = \bar{X}_2 + \bar{X}_3$$

- Good measurement equation, which does not hide the correlation

$$Y = \frac{\bar{X}_1 + \bar{X}_2}{\bar{X}_2 + \bar{X}_3}$$

Properties of a Good Measurement Equation Revisited

- A good measurement equation (ME) should:
  - Provide an adequate approximation to the value of the quantity of interest
  - Include an input value for every source of uncertainty
  - Be written in terms of the most fundamental measured quantities that will be used to compute the final value to avoid hidden correlations

Three Missteps Often Made in Uncertainty Evaluation

- Omitting significant sources of uncertainty in the measurement equation
- Not standardizing input uncertainties correctly, e.g., standard deviation used instead of standard error
- Including hidden correlations

Approaches to Measurement Uncertainty Calculation

- Assuming a good measurement equation and assuming good estimates for the input quantities values and uncertainties, how should one go about performing the calculations?
- The most direct way is to use calculus to determine the respective partial derivatives and then combine them by the laws of uncertainty propagation.
- This is the analytical approach.

Analytical Approach to Measurement Uncertainty Calculations

- Pros:
  - The most direct approach
  - Does not use approximations for partial derivative values
  - "Hands-on" approach
  - Can be accomplished with any calculation tool or even with pen and paper

- Cons:
  - Very time-intensive
  - Very prone to errors in calculating partial derivative values
  - Easy to miss correlations in the inputs

Numerical Approach to Measurement Uncertainty Calculation

- There are a number of software packages that will perform measurement uncertainty calculations using numerical approximations for the partial derivative values.

- These packages greatly facility the calculation of combined standard uncertainties.

- The analyst inputs the measurement equation, the values of the inputs, and the standard uncertainties of the inputs. The software then performs the calculations and outputs the results.

Software Packages for Measurement Uncertainty Calculations

- Kragten Spreadsheet
  - Excel spreadsheet developed by NIST based on the Kragten computational method
  - Available free from NIST
  - Does not have the "bells and whistles" of other packages
  - Limited to 15 inputs without modifying the spreadsheet

GUM Work Bench

- Sold by Metrodata GmbH
- Developed by Dr. Ruediger Kessel
- Well-written commercial software with many "bells and whistles"
- Widely used in the international nuclear community

Numerical Approach to Uncertainty Calculation

- Pros:
  - Automates calculations
  - Reduces calculation and transcription errors
  - Rapid results

- Cons:
  - Certain measurement functions do not lend themselves to accurate numerical differentiation
  - "Black box" approach hinders understanding of the uncertainty calculation process for the analyst
  - Quality of outputs is dependent on the quality and suitability of the inputs

Monte Carlo Approach to Measurement Uncertainty Calculations

- Uses computer simulation to estimate measurement uncertainties
- Pros:
  - Avoids differentiation issues
  - In some cases only approach that can give meaningful results
- Cons:
  - Not as widely used as other approaches
  - Sensitive to statistical models used for inputs
  - Does not easily generate an uncertainty budget
  - Heavy use of computer resources
- My experience with this approach is limited, so any further discussion of this topic is out of scope

Interpretation of GUM Results

- The expanded uncertainty is a numerical interval centered around the measured value in which, with a high degree of probability (chosen by the analyst; usually 95% or 99%), the actual value of the measurand is contained.

Uncertainty Budget

- Other than the combined standard uncertainty value, the uncertainty budget is the most import output from a GUM analysis
- The uncertainty budget, at a minimum, should contain the following for each measurement equation input:
  - Name of the input, its value, the units of the value, the standard uncertainty, the statistical model or distribution of the input, the partial derivative of the measurement equation with inspect to the input (sensitivity factor), the uncertainty contribution (the standard uncertainty multiplied by the sensitivity factor), and the contribution of the input to the overall squared uncertainty (index) (this is the uncertainty contribution squared, divided by the sum of all uncertainty contributions squared)

Uncertainty Budget Example

Quantity	Value	Units	Standard Uncertainty	Distribution	Sensitivity Coefficient	Uncertainty Contribution	Index
dg_ave	0.9993176 g U/g Sample	g U/g Sample	55.0E-6 g U/g Sample	normal	-1	-55E-6 g U/g Sample	67.90%
\delta_CRM112a	1.000000		3.00E-05	normal	-1	-30E-6 g U/g Sample	20.20%
certval	0.9997700 g U/g Sample	g U/g Sample	23.0E-6 g U/g Sample	normal	1	23E-6 g U/g Sample	11.90%
dif	452.4E-6 g U/g Sample	g U/g Sample	66.7E-6 g U/g Sample				
Squared Combined Uncertainty						4.454E-09	
Standard Combined Uncertainty		6.67383E-05					

Value of the Uncertainty Budget

- Information – it indicates which inputs are significant contributors to the overall uncertainty and which have negligible impact
- Diagnostic – are the major contributors expected? Are any major contributors unanticipated? If so, it may indicate a problem with the measurement equation or the values of the inputs' standard uncertainties
- Quality – are the major contributors type A? Are any major contributors values subjective or not reliable? If so, you may need to reevaluate your methods for estimating the standard uncertainties of these inputs or understand that the expanded uncertainty on your measurand is not reliable

Example Measurement Uncertainty Evaluation

- **D&G Titration**

- Purpose: The determination of elemental uranium concentration in single replicate of a solution using Davies & Gray titration (D&G titration)

Measurement Equation

- $U_{Assay,solution} = TEF * \underline{M}_{Titrant,sample} \underline{/ M}_{Solution,sample}$
- Where
  - $U_{Assay,solution}$ is the measurand, grams uranium per gram of solution
  - TEF – the titrant equivalency factor in g u per g titrant
  - $\underline{M}_{Titrant,sample}$ $\underline{, M}_{Solution,sample}$ - the masses of the titrant used and the mass of the sample solution in g

Inputs

- TEF: it is assumed that the titrant equivalency factor (Type A) for the titration system is 3.08183 mg/g with a standard uncertainty of 0.00013 mg/g (based on previous measurements of the TEF); converting to g/g, the value is 0.00308183 g/g with a standard uncertainty of 0.00000013g/g

Inputs

- $M_{Titrant,sample}$ value of 7.2930 g
- $M_{Solution,sample}$ value of 0.5994 g

- Both mass measurements have standard uncertainty of 0.000073 g (Type A, pooled estimate from 175 QA data points for the balance)

Results

Quantity	Value	Unit	Standard Uncertainty	Expanded Uncertainty	Unit	Coverage Factor	Coverage Confidence	
U Assay	0.0374971	g/g	0.0000049	0.0000097	g/g	2	95%	(normal)

Thus, the result may be expressed as
U Assay = 0.0374971 ± 0.0000097 g U/g Solution

Or to express as a percentage
U Assay = 3.74971 ± 0.00097 g U/g Solution, %

Uncertainty Budget

Quantity	Value	Standard Uncertainty	Distribution	Sensitivity Coefficient	Uncertainty Contribution	Index
TEF	3.081830E-3 g/g	130E-9 g/g	normal	12.2	1.6E-6 g/g	10.60%
$M_{Titrant}$	7.2930000 g	73.0E-6 g	normal	5.10E-03	380E-9 g/g	0.60%
$M_{Solution}$	0.5994000 g	73.0E-6 g	normal	-0.063	-4.6E-6 g/g	88.80%
U_{Assay}	0.03749714 g/g	4.85E-6 g/g				

What information can be drawn from the uncertainty budget?

Summary

- GUM is a comprehensive methodology to present measurement results in a consistent and coherent manner. It has increased the value of measurement reports.

- An institution cannot take adaption of GUM lightly. It requires commitment from its measurement staff, its data evaluators, and its management. GUM is as much a voyage as it is a manner of reporting measurements.

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Some slides and examples were adapted from various workshops led by Dr. Kattathu Mathew, New Brunswick Laboratory Senior Scientist, in 2009.

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Questions?

Upcoming NAMP Radiochemistry Webinars

- Mass Spectrometry (February 27)
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