AQR: Process of Estimating Uncertainty

NIST's eight-step process of estimating uncertainty

7.6.1.1.b-c AR
7.6.3
7.8.5
7.8.6.1
7.8.6.2

The following steps recommended by NIST will be used to estimate the uncertainty for each critical measurement in the laboratory:

- specify the measurement process
- identify and characterize the uncertainty sources
- quantify uncertainty estimates
- convert factors to standard uncertainties
- calculate combined standard uncertainty
- expand the uncertainty by **k**
- evaluate the expanded uncertainty
- report the uncertainty

The following explains how these steps are to be applied.

Step 1: specify the measurement process

In most cases, the evaluation of the measurement process will simply be identifying the type of measurement (for example, balance) in order to produce the formula for calculating the "combined total uncertainty". In the U.S., the method used is 'root sum squared' which is:

$$u_c = \sqrt{u_s^2 + s_p^2 + u_0^2 + u_2^2 + \ldots + u_i^2}$$

u_s^2 = uncertainty of reference standard
s_p^2 = standard deviation of measurement process
u_0^2 - u_i^2 = uncertainty contributors

Step 2: identify and characterize uncertainty sources

7.6.1

The next step is to identify all of the contributors to the total uncertainty of the measurement.

This should be accomplished by the formation of an uncertainty budget. The contribution (negligible to major) of each element must also be evaluated. This can be demonstrated through the use of diagrams, charts, or tables.

In cases where the measurement is a process of multiple steps and/or contains uncertainty contributions that cannot be quantified (for example, use of external data such as barometric pressure), the standard deviation of the entire measurement will be considered adequate for the standard deviation and the uncertainty contributors as it encompasses the uncertainty for all stages.

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Step 3: quantify uncertainty measurements

The next step is to assign a numerical value to each contributor.

For masses, the uncertainty is reported on the verification documentation for the standard. Instruments will have the uncertainty provided by the manufacturer in the instrument documentation.

The largest contributor to the uncertainty will usually be the "standard deviation of the measurement process". The source of this uncertainty is the analysts performing the measurement.

NIST states that the standard deviation calculation requires a minimum of seven data points with greater than 30 being preferred. However, an upper limit of diminishing returns can be reached at which time additional measurements no longer affect the calculation.

The standard deviation may be quantified in the following ways:

- using historical data from calibration checks or proficiency tests to establish a preliminary value
- having each analyst perform a measurement to evaluate repeatability and reproducibility
  - Repeatability is making the same measurement several times in a short period of time.
  - Reproducibility is making the same measurement in the same conditions at different times.
    - This compensates for environmental and other uncontrollable variables.

Step 4: Convert factors to standard uncertainties

In order to calculate the combined total uncertainty, all factors to be considered must be reduced to standard uncertainties.

The following divisors will be used:

- Normal: 1
- Rectangular: 1.7321
- Triangular: 2.4495

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Step 5: Calculate the combined standard uncertainty

The combined standard uncertainty will be calculated using the "root sum squared" method; square each contributor to the uncertainty, add the squares and take the square root of the total. Refer to *Step 1* for the formula.

Step 6: expand the uncertainty

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7.8.3.1.c).1 AR

The calculated uncertainty is then expanded to the desired confidence level. This is achieved by multiplying the combined standard uncertainty (u_c) by the coverage factor (k): $U = k*u_c$

- For approximately 95% (95.45%) confidence, multiply the combined standard uncertainty by **2.**
- For approximately 99% (99.73%) confidence, multiply the combined standard uncertainty by **3**.

Step 7: evaluate the uncertainty

The next step is to evaluate the number to determine if the value seems too large or too small based on the contributing factors. This is designed to catch any possible calculation errors. There are no strict criteria for this evaluation.

Step 8: report the uncertainty

7.8.3.1.a-e
7.8.1.1.c).1 AR

The final step is to report the uncertainty.

- The uncertainty typically has better resolution than the measurement itself.
- The uncertainty should be rounded to 2 significant digits and the result of the measurement should be reported to the same number of decimal places as the uncertainty is reported.
- The uncertainty components must be identified and the rationale included.

Example: "The mass of the methamphetamine was 9.72 g +/- 0.03 g. The reported uncertainty is expanded using a coverage factor of k=2 for a level of confidence of approximately 95%, assuming a normal distribution."