Designation: D7440 − 23

Standard Practice for Characterizing Uncertainty in Air Quality Measurements[1]

This standard is issued under the fixed designation D7440; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ε) indicates an editorial change since the last revision or reapproval.

1. Scope

1.1 This practice is for assisting developers and users of air quality methods for sampling concentrations of both airborne and settled materials in characterizing measurements as to uncertainty. Where possible, analysis into uncertainty components as recommended in the International Organization for Standardization (ISO) Guide to the Expression of Uncertainty in Measurement (ISO GUM, (**1**)[2]) is suggested. Aspects of uncertainty estimation particular to air quality measurement are emphasized. For example, air quality assessment is often complicated by: the difficulty of taking replicate measurements owing to the large spatio-temporal variation in concentration values to be measured; systematic error or bias, both corrected and uncorrected; and the (rare) non-normal distribution of errors. This practice operates mainly through example. Background and mathematical development are relegated to appendices for optional reading.

1.2 The values stated in SI units are to be regarded as standard. No other units of measurement are included in this standard.

1.3 *This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety, health, and environmental practices and determine the applicability of regulatory limitations prior to use.*

1.4 *This international standard was developed in accordance with internationally recognized principles on standardization established in the Decision on Principles for the Development of International Standards, Guides and Recommendations issued by the World Trade Organization Technical Barriers to Trade (TBT) Committee.*

2. Referenced Documents

2.1 *ASTM Standards:*[3]

D1356 Terminology Relating to Sampling and Analysis of Atmospheres

D3670 Guide for Determination of Precision and Bias of Methods of Committee D22

D6246 Practice for Evaluating the Performance of Diffusive Samplers

D6552 Practice for Controlling and Characterizing Errors in Weighing Collected Aerosols

2.2 *ISO Standards:*[4]

ISO GUM Guide to the Expression of Uncertainty in Measurement, ISO Guide 98, 1995 [5]

ISO 7708 Air Quality — Particle Size Fraction Definitions for Health-Related Sampling

ISO 15767 Workplace Atmospheres — Controlling and Characterizing Errors in Weighing Collected Aerosol

ISO 16107 Workplace Atmospheres — Protocol for Evaluating the Performance of Diffusive Samplers

ISO 16702 Workplace air quality — Determination of total organic isocyanate groups in air using 1-(2-methoxyphenyl)piperazine and liquid chromatography

3. Terminology

3.1 *Definitions*—For definitions of terms used in this practice, see Terminology D1356.

3.2 *Other Terms Defined as Follows are Taken from ISO GUM, Unless Otherwise Noted:*

3.2.1 *accuracy*—closeness of agreement between the result of a measurement and a true value of the measurand.

3.2.2 *combined standard uncertainty, u_c*—standard uncertainty of the result of a measurement when that result is

[1] This practice is under the jurisdiction of ASTM Committee D22 on Air Quality and is the direct responsibility of Subcommittee D22.01 on Quality Control.

Current edition approved Sept. 1, 2023. Published October 2023. Originally approved in 2008. Last previous edition approved in 2015 as D7440 – 08 (2015)$^{\varepsilon1}$. DOI: 10.1520/D7440-23.

[2] The boldface numbers in parentheses refer to the list of references at the end of this standard.

[3] For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.

[4] BIPM version available for download from http://www.bipm.org/en/publications/guides/gum.html. ISO version available from American National Standards Institute (ANSI), 25 W. 43rd St., 4th Floor, New York, NY 10036, http://www.ansi.org.

[5] See Ref (**1**), for an additional measurement uncertainty resource.

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 covariances of these other quantities weighted according to how the measurement result varies with changes in these quantities.

3.2.2.1 *Discussion*—As within ISO GUM, the "other quantities" are designated uncertainty components u_j from source j. The component u_j is taken as the standard deviation estimate from source j in the case of a source of random variation.

3.2.3 *coverage factor, k*—numerical factor used as a multiplier of the combined standard uncertainty (u_c) in order to obtain an expanded uncertainty (U).

3.2.3.1 *Discussion*—The factor k depends on the specific meaning attributed to the expanded uncertainty U. However, for simplicity this practice adopts the now nearly traditional coverage factor as the value 2, determining the specific meaning of the expanded uncertainty U in different circumstances. Other coverage factors if needed are then easily implemented simply by multiplication of the traditional expanded uncertainty U (see 7.1 – 7.4).

3.2.3.2 *Discussion*—The use of a single coverage factor, often through approximation, avoids the overly conservative use of individual component confidence limits rather than root variance estimates as uncertainty components.

3.2.4 *error (of measurement)*—result of a measurement minus a true value of the measurand.

3.2.5 *expanded uncertainty, U*—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.

3.2.5.1 *Discussion*—This definition has the breadth to encompass a wide variety of conceptions.

3.2.5.2 *Discussion*—The expanded uncertainty U in some cases is expressed in absolute terms, but sometimes as relative to the measurement result. What is meant is generally clear from the context.

3.2.6 *influence quantity*—quantity that is not the measurand but that affects the result of the measurement.

3.2.7 *measurand*—particular quantity subject to measurement.

3.2.8 *measurand value*—(adapted from ISO GUM), unknown quantity whose measurement is sought, often called the true value.

3.2.8.1 *Discussion*—Examples are the concentration (mg/m^3) of a substance in the air at a particular time and place, the time-weighted average of a concentration at a particular position, or the expected mean concentration estimate as obtained by a reference method at a specific time and position.

3.2.9 *(population) variance (of a random variable)*—the expectation of the square of the centered random variable.

3.2.10 *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 the same (*repeatability*) conditions of measurement.

3.2.10.1 *Discussion*—Random error is equal to error minus systematic error.

3.2.11 *(sample) variance*—the sum of the squared deviations of observations from their average divided by one less than the number of observations.

3.2.11.1 *Discussion*—The sample variance is an unbiased estimator of the population variance.

3.2.12 *standard deviation*—positive square root of the variance.

3.2.13 *symmetric accuracy range A*—the range symmetric about (true) measurand values containing 95 % of measurement estimates.

3.2.13.1 *Discussion—A* is a specific quantification of *accuracy* (**2**). **ISO 16107**

3.2.14 *systematic error (bias)*—mean that would result from an infinite number of measurements of the same measurand carried out under repeatability conditions minus a true value of the measurand.

3.2.15 *Type A evaluation (of uncertainty)*—method of evaluation of uncertainty by the statistical analysis of series of observations.

3.2.16 *Type B evaluation (of uncertainty)*—method of evaluation of uncertainty by means other than the statistical analysis of series of observations.

4. Background Information

4.1 Uncertainty in a measurement result can be taken as the range about an estimate, corrected for bias if known, containing the true, or mean reference value—in the language of ISO GUM, the *measurand* value at given confidence. Uncertainty accounts not only for variation in a method's results at application, but also for incomplete characterization of the method when evaluated. In accordance with ISO GUM, uncertainty may often usefully be analyzed into individual components.

4.2 There are several aspects of uncertainty characterization specific to air quality measurements. One of these aspects concerns known, that is, correctible, systematic error or mean bias of a measurement relative to a true measurand value. Several measurement methods exist with such bias left uncorrected because of policy, tradition, or other reason. *Uncertainty* deals only with what is unknown about a measurement, and as such does not include correctible (known) bias. The magnitude of the difference between estimate and measurand value is covered by *accuracy* as defined qualitatively in ISO GUM, rather than *uncertainty*, particularly when the bias is known, but uncorrected. Such methods require specification of both uncertainty and as much as is known of the uncorrected bias, or alternatively the adoption of an accuracy measure.

4.3 Often bias is known to exist, but with unknown value. In the case where only limits may be placed on the magnitude of the bias, ISO GUM generally recommends treating the bias as uniformly distributed within the known limits. Such a distribution refers to independent situations, for example, calibrations, where bias may arise (see 7.4 and Appendix X2), rather than variation at the point of method application. Even though such an equal-likelihood bias distribution may be unrealistic, nevertheless a standard deviation estimate may be