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# Air quality — Guidelines for estimating measurement uncertainty

*Qualité de l'air — Lignes directrices pour estimer l'incertitude de mesure*



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# Foreword

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International Standards are drafted in accordance with the rules given in the ISO/IEC Directives, Part 2.

The main task of technical committees is to prepare International Standards. Draft International Standards adopted by the technical committees are circulated to the member bodies for voting. Publication as an International Standard requires approval by at least 75 % of the member bodies casting a vote.

Attention is drawn to the possibility that some of the elements of this document may be the subject of patent rights. ISO shall not be held responsible for identifying any or all such patent rights.

ISO 20988 was prepared by Technical Committee ISO/TC 146, *Air quality*, Subcommittee SC 4, *General aspects*.

## Introduction

The general concept of uncertainty estimation is described in the *Guide to the Expression of Uncertainty in Measurement* (GUM). Practical considerations of the GUM are focussed on evaluation of series of unbiased observations. In air quality measurements, series of observations may rarely be considered unbiased due to the presence of random effects not varying throughout a series of observations.

This International Standard supports evaluation of random effects causing variation or bias in series of observations for the purpose of uncertainty estimation. Appropriate data may be collected in experimental designs providing comparison with reference material, or with reference instruments, or with independent measurements of the same type. In provision of experimental data for uncertainty estimation, it is important to ensure representativeness for variations and bias occurring in intended use of the method of measurement.

Generic guidance and statistical procedures presented by this International Standard are addressed to technical experts of air quality measurement, acting, e.g. in standardization, validation or documentation of methods of measurement in ambient air, indoor air, stationary source emissions, workplace atmospheres or meteorology.

This International Standard does not provide comprehensive information on planning and execution of experimental designs to be evaluated for the purpose of uncertainty estimation.



Uncertainties of results of measurement caused by incomplete time-coverage of measurement data are not considered in this document, but in ISO 11222[2]. Uncertainties of results of measurement induced by incomplete spatial coverage by measurement data are not considered in this document.

# Air quality — Guidelines for estimating measurement uncertainty

## 1 Scope

This International Standard provides comprehensive guidance and specific statistical procedures for uncertainty estimation in air quality measurements including measurements of ambient air, stationary source emissions, indoor air, workplace atmospheres and meteorology. It applies the general recommendations of the *Guide to the Expression of Uncertainty in Measurement* (GUM) to boundary conditions met in air quality measurement. The boundary conditions considered include measurands varying rapidly in time, as well as the presence of bias in a series of observations obtained under conditions of intended use of methods of air quality measurement.

The methods of measurement considered comprise

— methods corrected for systematic effects by repeated observation of reference materials,

— methods calibrated by paired measurement with a reference method,

— methods not corrected for systematic effects because they are unbiased by design, and

— methods not corrected for systematic effects in intended use deliberately taking into account a bias.



Experimental data for uncertainty estimation can be provided either by a single experimental design in a direct approach or by a combination of different experimental designs in an indirect approach.

## 2 Normative references

The following referenced documents are indispensable for the application of this document. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

ISO/IEC Guide 98:1995, *Guide to the expression of uncertainty in measurement (GUM)*

## 3 Terms and definitions

**3.1**
**uncertainty (of measurement)**
**measurement uncertainty**
parameter, associated with the result of a measurement, that characterizes the dispersion of the values that could reasonably be attributed to the measurand

[ISO/IEC Guide 98:1995, B.2.18; VIM:1993, 3.9]

**3.2**
**standard uncertainty**
uncertainty of the result of measurement expressed as a standard deviation

[ISO/IEC Guide 98:1995, 2.3.1]

NOTE The standard uncertainty of a result of measurement is an estimate of the standard deviation of the population of all possible results of measurement which can be obtained by means of the same method of measurement for the measurand exhibiting a unique value.

**3.3**
**combined standard uncertainty**
standard uncertainty of the result of measurement when that result is obtained from the values of a number of other input quantities, equal to the positive square root of a sum of terms, the terms being the variances or covariance of these other quantities weighted according to how the measurement result varies with changes in these quantities

[ISO/IEC Guide 98:1995, 2.3.4]

NOTE The adjective “combined” can be omitted often without loss of generality.

**3.4**
**expanded uncertainty**
quantity defining an interval $[y - U_p(y); y + U_p(y)]$ about the result of a measurement $y$ that may be expected to encompass a large fraction $p$ of the distribution of values that could reasonably be attributed to the measurand

NOTE 1 Adapted from ISO/IEC Guide 98:1995, 2.3.5.

NOTE 2 If the uncertainty has been obtained mainly by Type A evaluation, the interval $[y - U_p(y); y + U_p(y)]$ can be understood as confidence interval for the true value of the measurand on a level of confidence $p$.

NOTE 3 The interval $[y - U_p(y); y + U_p(y)]$ characterizes the range of values within which the true value of the measurand is confidently expected to lie (see ISO/IEC Guide 98:1995, 2.2.4).



**3.5**
**coverage factor**
numerical factor used as multiplier of the combined standard uncertainty in order to obtain an expanded uncertainty



[ISO/IEC Guide 98:1995, 2.3.6]

**3.6**
**coverage probability**
fraction of results of measurement expected to be encompassed by a specified interval

**3.7**
**Type A evaluation (of uncertainty)**
method of evaluation of uncertainty by the statistical analysis of series of observations

[ISO/IEC Guide 98:1995, 2.3.2]

**3.8**
**Type B evaluation (of uncertainty)**
method of evaluation of uncertainty by means other than the statistical analysis of series of observations

[ISO/IEC Guide 98:1995, 2.3.3]

**3.9**
**standard deviation**
positive square root of the variance

[ISO/IEC Guide 98:1995, C.2.12]

NOTE In general, the standard deviation of the population of a random variable $X$ is estimated by the positive square root of an estimate of the variance of the population of $X$.

**3.10**
**experimental standard deviation**
for a series of $N$ measurements of the same measurand, the quantity $s(x)$ characterizing the dispersion of the results is given by the formula

$$s(x) = \sqrt{\sum_{j=1}^{N} \frac{\left(x(j) - \bar{x}\right)^2}{N-1}}$$

$x(j)$ being the result of the $j$th measurement and $\bar{x}$ being the arithmetic mean of the $N$ results considered

NOTE 1 Adapted from ISO/IEC Guide 98:1995, B.2.17.

NOTE 2 $s^2(x)$ is an unbiased estimate of the variance $\sigma^2(X)$ of the investigated random variable $X$, if the series of observations $x(j)$ with $j = 1$ to $N$ is unbiased.

**3.11**
**variance**
the expectation of the square of the centred random variable:

$$\sigma^2(X) = E\left\{\left[X - E(X)\right]^2\right\}$$

[ISO/IEC Guide 98:1995, C.2.11]

NOTE The population variance $\sigma^2(X)$ of a random variable $X$ can be estimated by the square of the experimental standard deviation $s^2(x)$ of a simple random sample of unbiased observations $x(j)$ with $j = 1$ to $N$ of the random variable $X$. Otherwise, $s^2(x)$ underestimates the population variance.



**3.12**
**covariance**
mean of the product of two centred random variables in their joint probability distribution



NOTE 1 Adapted from ISO 3534-1: 2006, 2.43.

NOTE 2 The covariance cov($x$, $y$) is a sample statistic used to estimate the covariance of the populations of $x$ and $y$.

**3.13**
**expectation**
**expected value**

1) For a discrete random variable $X$ taking the values $x_i$ with probabilities $p_i$, the expectation, if it exists, is $E(X) = \Sigma\, p_i\, x_i$, the sum being extended over all values $x_i$ which may be taken by $X$.

2) For a continuous random variable $X$ having the probability density function $f(x)$, the expectation, if it exists, is $E(X) = \int x \cdot f(x) \cdot \mathrm{d}x$, the integral being extended over the interval(s) of variation of $X$.

[ISO/IEC Guide 98:1995, C.2.9]

**3.14**
**degrees of freedom**
in general, the number of terms in a sum minus the number of constraints on the terms of the sum

[ISO/IEC Guide 98:1995, C.2.31]

NOTE For a variance estimate, the (effective) number of degrees of freedom can be understood as the number of independent pieces of information used to obtain that variance estimate.

**3.15**
**measurement**
set of operations having the object of determining the value of a quantity

[VIM:1993, 2.1]

**3.16**
**result of measurement**
value attributed to the measurand, obtained by measurement

[VIM:1993, 3.1]

**3.17**
**sensitivity coefficient**
deviation of the result of measurement divided by the deviation of an influence quantity causing the change, if all other influence quantities are kept constant

**3.18**
**measurand**
particular quantity subject to measurement

[VIM:1993, 2.6]

NOTE The measurand is considered to exhibit a unique value at least for the time period needed for a single measurement.

**3.19**
**measuring system**
complete set of measuring instruments and other equipment with operating procedures to carry out specified air quality measurements

[ISO 11222:2002, 3.9]



NOTE A measuring system is a technical realization of a method of measurement. Method documentation is considered part of a measuring system.



**3.20**
**reference material**
**RM**
material or substance for which one or more properties are sufficiently homogeneous and well established to be used for the calibration and/or the validation of a measuring system

NOTE 1 Adapted from VIM:1993, 6.13.

NOTE 2 A reference material may be in the form of a pure or mixed gas, liquid or solid.

**3.21**
**systematic effect**
Influence causing a bias that is expected to occur consistently in each series of observations obtained in repeated or parallel execution of the measurement

**3.22**
**random effect**
influence causing either random variation or a bias of random value (inconsistent bias) in a series of observation obtained in repeated execution of the measurement

NOTE An effect exhibiting a fixed, but random value while executing the measurement repeatedly causes a bias of random value.

**3.23**
**bias**
systematic error of the indication of a measuring instrument

[VIM:1993, 5.25]

NOTE A bias of a series of observations about an accepted reference value can be caused either by systematic effects, or by random effects exhibiting (unknown) fixed values in the series of observations.

 

**3.24**
**representativeness**
ability of a series of observations to provide an unbiased estimate of a parameter of a specified statistical population

**3.25**
**population**
totality of items under consideration

[ISO 3534-1:2006, 1.1]

NOTE Ensemble of possible results of measurement which can be obtained for a unique measurand by all possible technical realizations of a specified method of measurement.

## 4 Symbols and abbreviated terms

| | |
|---|---|
| $a$ | parameter (constant) |
| $b$ | parameter (constant) |
| $c$ | parameter (constant) |
| $c_i$ | sensitivity coefficient |
| $\mathrm{cov}(x_i, x_k)$ | estimate of covariance between input quantities $x_i$ and $x_k$ |
| $E(X)$ | expectation of random variable $X$ |
| $i$ | index |
| $j$ | index |
| $k$ | index |
| $k_p$ | coverage factor |
| $K$ | number |
| $L$ | number of laboratories |
| $M$ | number |
| $N$ | number |
| $p$ | coverage probability; level of confidence |
| $\sigma(x)$ | standard deviation of the population of a random variable $X$ |
| $s(x)$ | experimental standard deviation of data set $x(j)$ with $j = 1$ to $N$ |
| $t(p, \nu)$ | $(1 - p)$-quantile of Student's $t$-distribution of $\nu$ degrees of freedom |
| $u_\mathrm{B}$ | uncertainty caused by bias |
| $u(x_i)$ | standard uncertainty of input value $x_i$ |



 

$u(x_R)$ (combined) standard uncertainty of reference value $x_R$

$u(y_R)$ (combined) standard uncertainty of reference value $y_R$

$u(y_R(j))$ (combined) standard uncertainty of reference value $y_R(j)$

$U_p(y)$ expanded uncertainty of result of measurement $y$ on level of coverage $p$

var($x_i$) estimate of the variance of input quantity $x_i$

var($Y$) estimate of the variance of possible results of measurement $Y$

var($y$) estimate of the variance of results of measurement $y(j)$ with $j$ = 1 to $N$ observed in a direct approach

$w(y)$ relative standard uncertainty of a result of measurement $y$

$W_p(y)$ relative expanded uncertainty of a result of measurement $y$ on level of coverage $p$

$x_i$ input quantity of the method model equation $y = f(x_1,\ldots,x_K)$

$x_R$ reference value for input quantity $x$

$\delta X$ potential deviation of influence quantity $x$

$Y$ possible result of measurement that could reasonably be attributed to the same measurand by independent replication of the measurement which was executed to obtain the result of measurement $y$

$y$ result of measurement

$y_R$ accepted value of reference material of the measurand

$y_R(i)$ result of measurement obtained by a reference method of measurement

$\delta Y$ potential deviation of result of measurement $y$ about the (unknown) true value of the measurand, which is not described implicitly by the experimental data to be evaluated

$\gamma$ level of confidence

$\mu$ (unknown) true value of the measurand

$\nu$ number of degrees of freedom

$\nu_{eff}$ effective number of degrees of freedom

$\chi^2(\gamma, \nu)$ $\gamma$–percentile of chi-square distribution of $\nu$ degrees of freedom



## 5 Basic concepts

### 5.1 Outline

The general objective of this International Standard is to support application of the *Guide to the Expression of Uncertainty in Measurement* (GUM) in the various fields of air quality measurement including ambient air, indoor air, meteorology, stationary source emissions and workplace atmospheres. Standard methods of air quality measurement are considered to be fully documented, e.g. in method standards, standard operating procedures, validation reports or in other technical documents.

Documentation for a given method should comprise

— instructions on intended use (standard operating procedure),

— instructions on correction for systematic effects, if appropriate,

— method model equation $y = f(x_1,..., x_K)$, if results of measurement $y$ are calculated from observed or otherwise known input quantities $x_i$,

— results of method-validation, if appropriate, and

— instructions on how to assign uncertainty parameters to results of measurement $y$.

The focus of this International Standard is on how to assign appropriate uncertainty parameters to results of measurement obtained by air quality measurement methods. To this end, uncertainty estimation is considered to be a five-step procedure consisting of

— problem specification (see Clause 6),

— statistical analysis (see Clause 7),

— estimation of variances and covariances (see Clause 8),

— evaluation of uncertainty parameters (see Clause 9), and

— reporting (see Clause 10).

Figure 1 relates this five-step procedure to the eight steps recommended by the GUM.

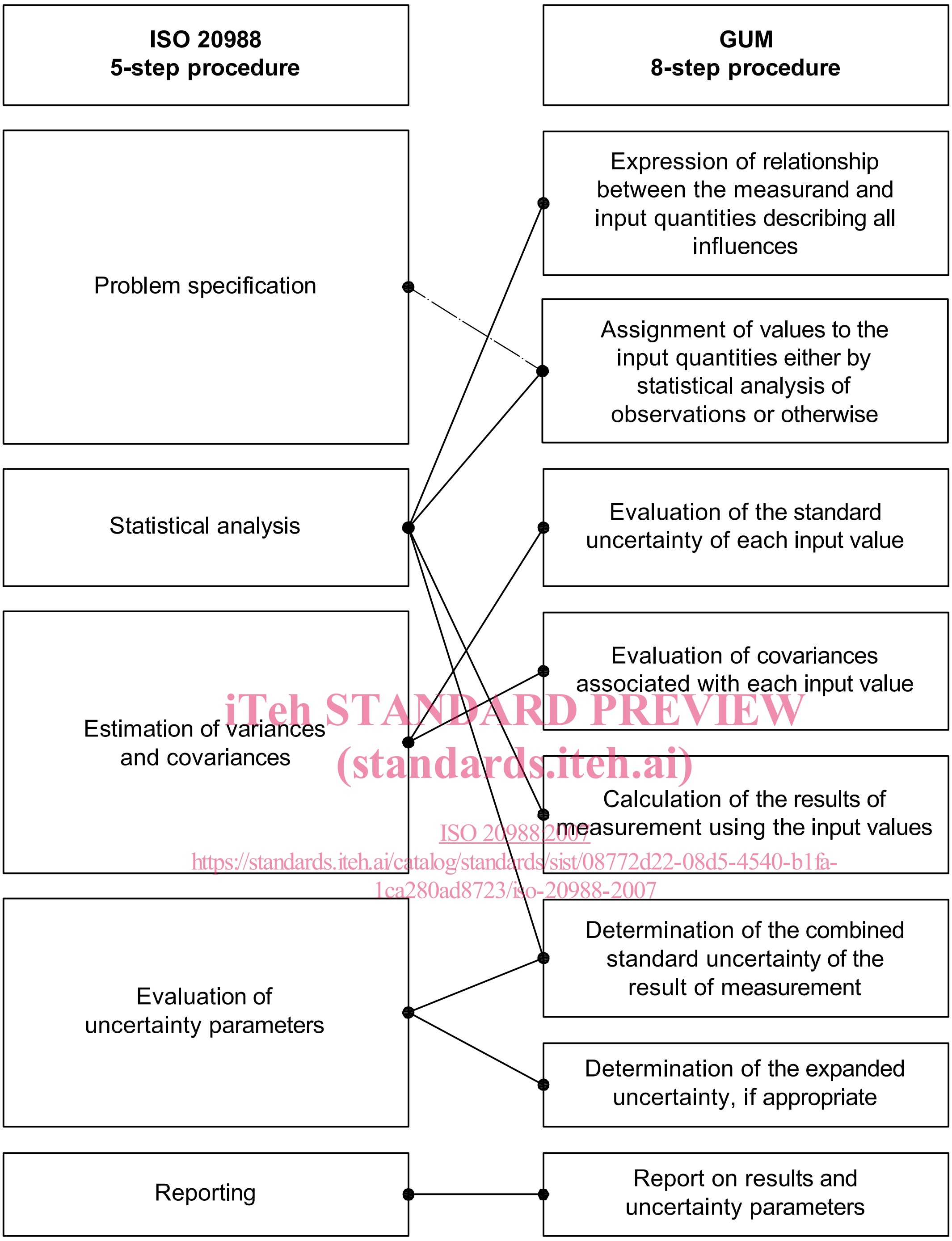




**Figure 1 — Comparison of the 5-step ISO 20988 procedure (left side) with the 8-step procedure of the GUM (right side)**

The main objectives of problem specification as a separate first step are

- to identify the questions to be answered, and
- to provide input data to be evaluated.

Starting from a proper problem specification, this International Standard provides guidance to statistical analysis and to evaluation methods which are applicable without mathematical expertise. Problem specification requires expert knowledge of technical aspects of the measurement considered and at least a basic understanding of the general statistical concept of uncertainty estimation described by the GUM. A brief introduction to the statistical aspects of uncertainty estimation is provided in 5.2, 5.3 and 5.4.

## 5.2 Measurement uncertainty

Measurement uncertainty is defined 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 3.1).

An appropriate uncertainty parameter can be:

- the (combined) standard uncertainty $u(y)$ of a result of measurement $y$;
- the expanded uncertainty $U_p(y)$ of a result of measurement $y$ on a specified level of coverage $p$.

In accordance with definition 3.1, the (combined) standard uncertainty $u(y)$ of a result of measurement $y$ is the positive square root of an estimate var($Y$) of the variance of the population of possible results of measurement $Y$ that could reasonably be attributed to the same measurand by independent replication of the measurement. Accordingly, a basic task in uncertainty estimation is to provide an estimate var($Y$) of the variance of the population of possible results of measurement $Y$. A detailed statistical discussion is provided in Clause 7.



Following definition 3.4, the expanded uncertainty $U_p(y)$ describes an interval $[y - U_p(y); y + U_p(y)]$ about a specific result of measurement $y$, which is expected to encompass a large fraction $p$ of the possible results that could reasonably be attributed to the same measurand by independent replication of the measurement. For a specified coverage probability $p$, the corresponding expanded uncertainty $U_p(y)$ is obtained as a multiple of the (combined) standard uncertainty $u(y)$. This implies a Gaussian distribution of possible results of measurement about the unique but unknown value of the measurand. For details, see 9.3.

The common understanding of an uncertainty interval $[y - U_p(y); y + U_p(y)]$ is that of an estimate characterizing the range of values within which the true value of the measurand lies (see ISO/IEC Guide 98:1995, 2.2.4), i.e. within which the value of the measurand is confidently believed to lie [4]. The coverage probability $p$ describes the degree of belief that the true value of the measurand is covered by the interval $[y - U_p(y); y + U_p(y)]$.

Given a specified expanded uncertainty $U_p(y)$ and an appropriate set of input data, the coverage probability $p$ of the uncertainty interval $[y - U_p(y); y + U_p(y)]$ about an observed result of measurement $y$ can be tested in a robust manner. This method does not imply a Gaussian distribution of possible results of measurement about the unknown value of the measurand. Details are given in Annex A.

If appropriate, the combined standard uncertainty $u(y)$ can be described as a function of the result of measurement $y$, e.g. $w(y) = u(y)/y$ = constant. An uncertainty function of this kind can be closely linked to a method model equation $y = f(x_1,..., x_K)$ used to obtain results of measurement $y$. This concept is illustrated by Figure 2.