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Australian/New Zealand Standard™

Air quality — Guidelines for estimating measurement uncertainty



AS/NZS ISO 20988:2024

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Australian/New Zealand Standard™

Air quality — Guidelines for estimating measurement uncertainty

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Preface

This Standard was prepared by the Joint Standards Australia/Standards New Zealand Committee EV-007, Methods for Examination of Air.

The objective of this document is to provide 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 include the following:

- (a) Methods corrected for systematic effects by repeated observation of reference materials.
- (b) Methods calibrated by paired measurement with a reference method.
- (c) Methods not corrected for systematic effects because they are unbiased by design.
- (d) 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.

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Foreword

ISO (the International Organization for Standardization) is a worldwide federation of national standards bodies (ISO member bodies). The work of preparing International Standards is normally carried out through ISO technical committees. Each member body interested in a subject for which a technical committee has been established has the right to be represented on that committee. International organizations, governmental and non-governmental, in liaison with ISO, also take part in the work. ISO collaborates closely with the International Electrotechnical Commission (IEC) on all matters of electrotechnical standardization.

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.

NOTES

Australian/New Zealand Standard

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

[SOURCE: 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

[SOURCE: ISO/IEC Guide 98:1995, 2.3.1]

Note 1 to entry: 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

[SOURCE: ISO/IEC Guide 98:1995, 2.3.4]

Note 1 to entry: 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 to entry: Adapted from ISO/IEC Guide 98:1995, 2.3.5.

Note 2 to entry: 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 to entry: 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

[SOURCE: 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

[SOURCE: 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

[SOURCE: ISO/IEC Guide 98:1995, 2.3.3]

3.9

standard deviation

positive square root of the variance

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

Note 1 to entry: 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

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

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

Note 1 to entry: Adapted from ISO/IEC Guide 98:1995, B.2.17.

Note 2 to entry: $s^2(x)$ 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:

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

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

Note 1 to entry: 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 to entry: Adapted from ISO 3534-1: 2006, 2.43.

Note 2 to entry: The covariance $\text{cov}(x, y)$ 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 $E(X) = \sum p_i x_i$, 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 $E(X) = \int x \cdot f(x) \cdot dx$, the integral being extended over the interval(s) of variation of X .

[SOURCE: 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

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

Note 1 to entry: 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

[SOURCE: VIM:1993, 2.1]

3.16**result of measurement**

value attributed to the measurand, obtained by measurement

[SOURCE: 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

[SOURCE: VIM:1993, 2.6]

Note 1 to entry: 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

[SOURCE: ISO 11222:2002, 3.9]

Note 1 to entry: 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 to entry: Adapted from VIM:1993, 6.13.

Note 2 to entry: 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 1 to entry: 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

[SOURCE: VIM:1993, 5.25]

Note 1 to entry: 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

[SOURCE: ISO-3534-1:2006, 1.1]

Note 1 to entry: 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
$\text{cov}(x_i, x_k)$	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 ν degrees of freedom
u_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
$\text{var}(x_i)$	estimate of the variance of input quantity x_i
$\text{var}(Y)$	estimate of the variance of possible results of measurement Y

$\text{var}(y)$	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 $y = f(x_1, \dots, x_K)$
x_R	reference value for input quantity x
δX	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
δY	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
γ	level of confidence
μ	(unknown) true value of the measurand
ν	number of degrees of freedom
ν_{eff}	effective number of degrees of freedom
$\chi^2(\gamma, \nu)$	γ -percentile of chi-square distribution of ν 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 $y = f(x_1, \dots, x_K)$, 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.

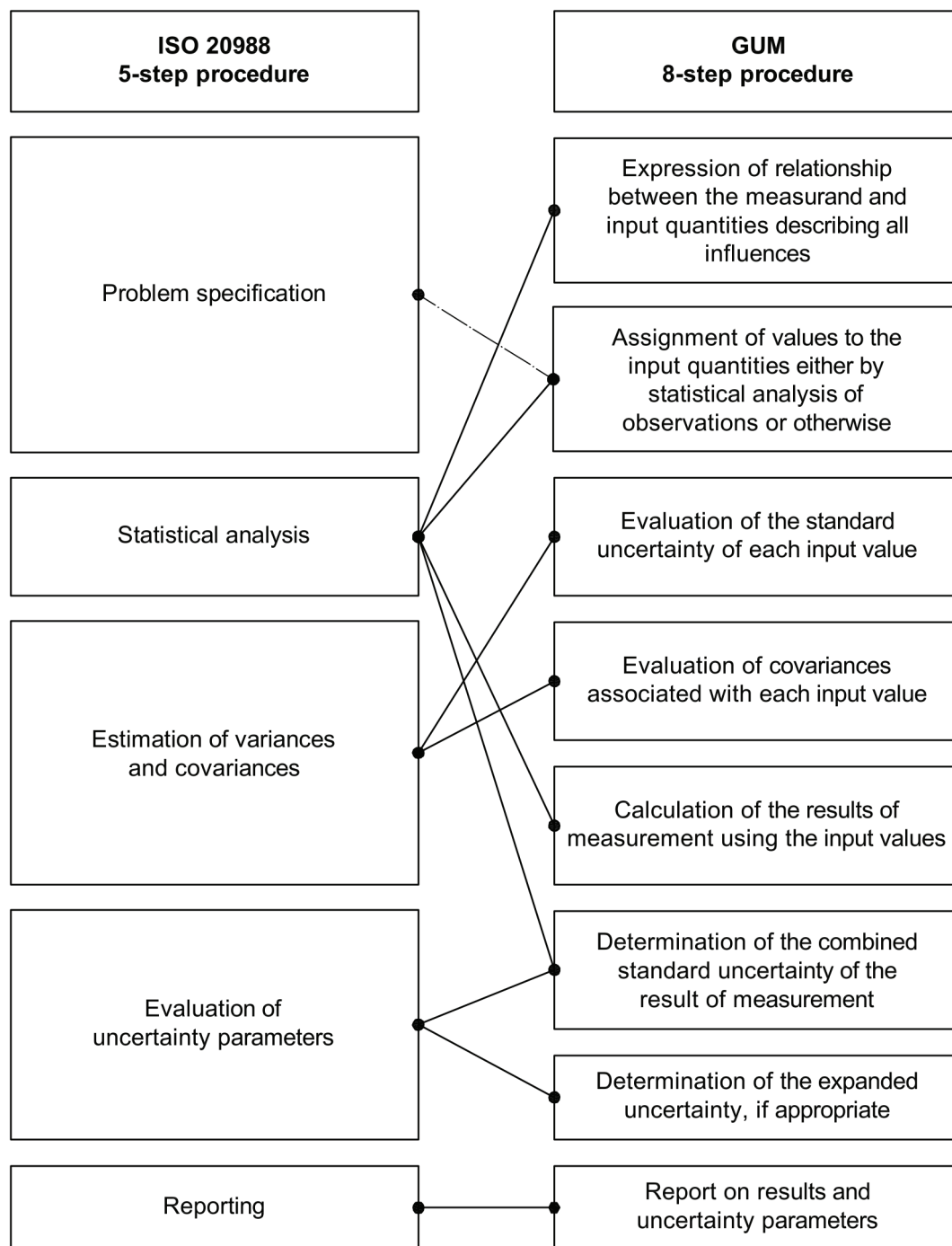


Figure 1 — Comparison of the 5-step ISO 20988 procedure (left side) with the 8-step procedure of the GUM (right side)

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 $\text{var}(Y)$ 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 $\text{var}(Y)$ 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. $w(y) = u(y)/y = \text{constant}$. An uncertainty function of this kind can be closely linked to a method model equation $y = f(x_1, \dots, x_K)$ used to obtain results of measurement y . This concept is illustrated by [Figure 2](#).

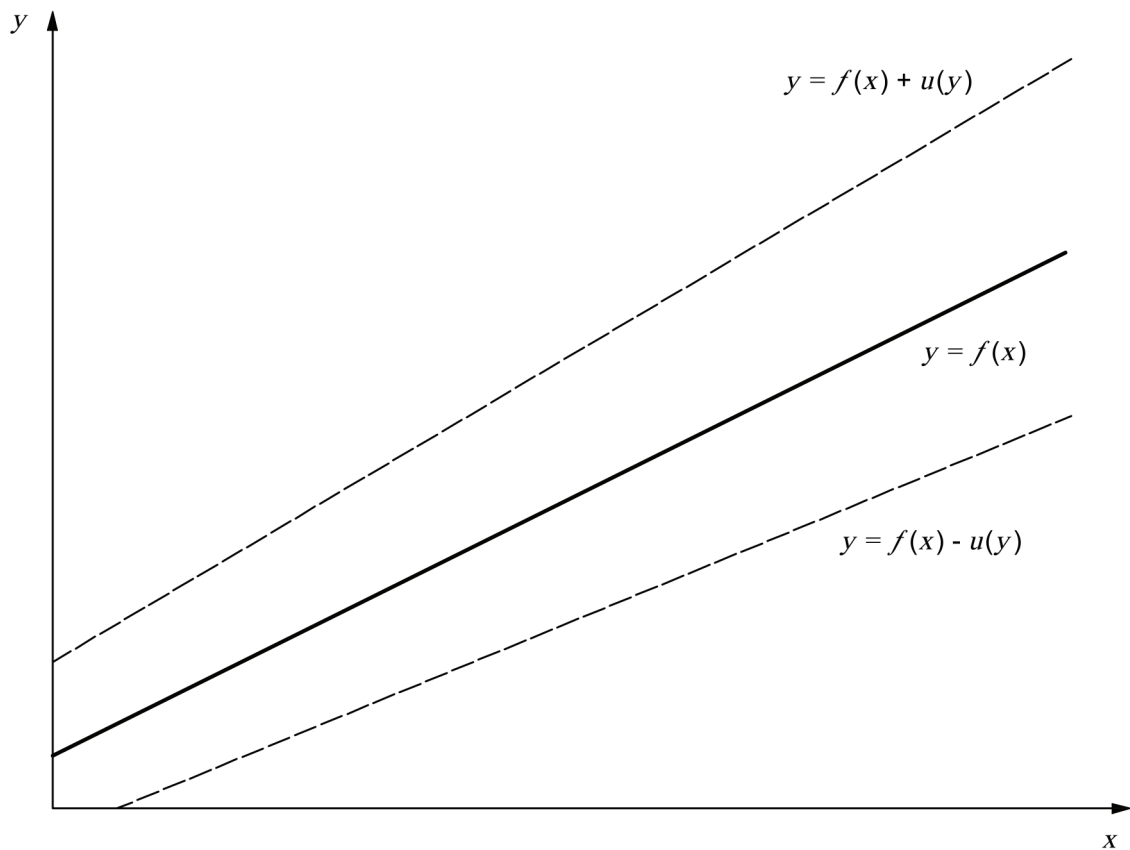


Figure 2 — Method model equation and uncertainty function

It is implicit in this International Standard that an uncertainty parameter obtained by evaluation of a specified set of input data shall be appropriate to predict the uncertainty of future results of measurement obtained by means of the same method of measurement under conditions represented by the input data evaluated. In order to ensure this, it is essential to provide supporting evidence that the evaluated input data are representative of the application of the method of measurement that will produce the results to be qualified by an uncertainty parameter.

5.3 Correction for systematic effects

Correction for systematic effects is an integral part of a measurement as far as required by the method documentation. In general, correction for systematic effects is achieved by comparison with one or more reference standards, e.g. in calibration or in drift control procedures. Appropriate reference standards can be provided by certified reference materials or by certified reference methods of measurement. By comparison with reference materials of SI units, traceability of possible results of measurement can be established. For a reference method being considered a primary measurement standard, comparison with other reference standards is not necessary for the purpose of correction.

It is a general recommendation of the GUM that corrections should be applied for all recognized significant systematic effects (see ISO/IEC Guide 98:1995, 3.2.4). In general, a correction procedure described by the method documentation can exhibit a certain degree of imperfection, e.g. due to its statistical character and due to the uncertainty of the reference standards used for this purpose. As an expression of the imperfection of a correction procedure, a series of corrected results of measurement obtained by the same measuring system can exhibit a residual bias, which is considered a random variable of expected value zero.

If a correction is applied in a measurement by means of a method model equation used to calculate the result of measurement, the uncertainty of the applied correction is taken into account properly.

If a bias is not corrected for, it shall be taken into account as an additional source of uncertainty.

In conclusion, for uncertainty estimation, it is necessary to collect series of observations that allow the user to evaluate both the variations and the bias occurring in the intended use of the method of measurement. If uncorrected significant bias was not taken into account, the estimation of measurement uncertainty is incomplete.

NOTE The terms "effect", "influence" and "source of uncertainty" are used with synonymous meaning in this International Standard.

5.4 Provision of input data

Input data for uncertainty estimation shall be representative of all effects causing variation or bias in results of measurement. Appropriate input data can be provided either by series of observations, or by external sources, or by expert judgement.

From a practical point of view, uncertainty estimation can be realized either in an indirect approach or in a direct approach.

In an indirect approach, variations and bias are, in a first step, evaluated separately for the input quantities x_i of the method model equation $y = f(x_1, \dots, x_K)$ used to obtain results of measurement y . For this purpose, estimates of the variances and covariances of the input quantities x_i can be provided by a Type A evaluation of series of observations or by a Type B evaluation based on expert judgement. Finally, a weighted sum of variances and covariances provides the wanted uncertainty estimate.

In a direct approach, the influences of the dominating effects causing variation and bias of the result of measurement y are investigated in a pooled way by comparison with one or more reference values of the measurand. Effects not varied in a direct approach shall be taken into account separately, e.g. by a Type B evaluation based on expert judgement. In a direct approach, the uncertainty estimation can be much simpler than in an indirect approach.

The focus of the GUM is on the indirect approach without excluding the direct approach.

The basic Type A evaluation method described by the GUM requires a series of unbiased observations of the same unchanged measurand obtained by the same measuring system. This experimental design is called simple random sampling. From a practical point of view, simple random sampling requires complete randomization of all effects between repeated observations of the same unchanged measurand. Simple random sampling is rarely realized under conditions of intended use of methods of air quality measurement, mainly due to the potential presence of uncorrected bias. The considerations of the GUM concerning a Type A evaluation are not exhaustive. There are many situations that can be treated by statistical methods different from the basic Type A evaluation described by the GUM (see ISO/IEC Guide 98:1995, 4.2.8).

In air quality measurements, it is often more convenient and cost-effective to provide input data for uncertainty estimation in experimental designs different from simple random sampling. In this International Standard, the following experimental designs are considered:

- A1: simple random sampling;
- A2: repeated observation of a reference material by a measuring system;
- A3: observation of different reference materials in a calibration procedure;
- A4: repeated observation of different reference materials by identical measuring systems;
- A5: parallel measurements with a reference method of measurement;
- A6: paired measurements of two identical measuring systems;
- A7: interlaboratory comparison of identical measuring systems;
- A8: parallel measurement of identical measuring systems.

The experimental designs of types A1 to A8 are applicable in indirect as well as in direct approaches for uncertainty estimation of methods of air quality measurement, comprising the following:

- methods of measurement corrected for systematic effects by (repeated) observation of reference material;
- methods of measurement evaluated by repeated observation of reference materials of the measurand prior to routine application;
- methods of measurement calibrated by parallel measurement with a reference method of measurement;
- methods of measurement verified by parallel measurement with a reference method of measurement;
- legal or other accepted reference methods of measurement validated by inter-comparison tests.

Appropriate series of observations can be provided, e.g. by one of the following procedures:

- QA/QC procedure applied repeatedly to the measuring system;
- verification procedure applied once to the measuring system;
- evaluation procedure applied to several measuring systems of the same type;
- validation procedure applied once to several measuring systems of the same type;
- another performance test applied to the measuring system.

Input data for uncertainty estimation can also be provided by external sources if these data are based on statistical evaluation of series of observations, such as accepted values and uncertainties of reference materials, values and uncertainties of instrument constants provided by independent reports or values and uncertainties of physical or chemical constants provided by handbooks (see ISO/IEC Guide 98:1995, 4.1.3).

NOTE The use of external data on reproducibility and trueness of a method of measurement that were obtained by application of ISO 5725-2[5], ISO 5725-3[6], ISO 5725-4[7] and ISO 5725-5[8] is described in ISO/TS 21748[9].

If input data cannot be provided as a series of observations or from an external source, such data can be obtained by expert judgement and evaluated by a method of Type B.

The applicability of an uncertainty parameter for future results of measurement obtained by the evaluated method of measurement depends on the representativeness of the input data. The degree of representativeness achieved by a set of input data depends on the following:

- effects described by the input data;
- sample size of the collected series of observations;
- uncertainty of the reference standards applied in this investigation.

The closer the input data describe all effects influencing the measurement, and the smaller the uncertainty of the reference standards, the better is the predictive power of an obtained uncertainty parameter for future results of measurement.

Of course, it is an important issue to test the predictive power of an uncertainty parameter, e.g. by another independent evaluation of measurement uncertainty.

For estimating an expanded uncertainty $U_{0,95}(y)$ on a level of confidence of 95 %, it is recommended to provide a series of observations comprising at least 20 applications of the specified method of measurement. Otherwise, the applicability of the obtained uncertainty parameter cannot be subjected to a meaningful test.

For estimating an expanded uncertainty $U_{0,66}(y)$ on a level of confidence of 66 %, it is recommended to provide a series of observations comprising at least seven applications of the specified method of measurement. Otherwise, the applicability of the obtained uncertainty parameter cannot be subjected to a meaningful test.

For details on the provision of input data and the applicable mathematical evaluation methods, see [6.4](#) and [8.2](#), respectively.

6 Problem specification

6.1 Objectives

The objective of problem specification in uncertainty estimation is to identify

- the measurement to be considered,
- the required uncertainty parameter,
- the input data to be evaluated, and
- the effects not described by input data.

[Figure 3](#) outlines the relationships between the elements of problem specification in uncertainty estimation. Problem specification requires expert knowledge of technical aspects of the measurement considered. Guidance provided in [6.2](#) to [6.4](#) is applicable without expertise in statistical modelling of measuring processes.

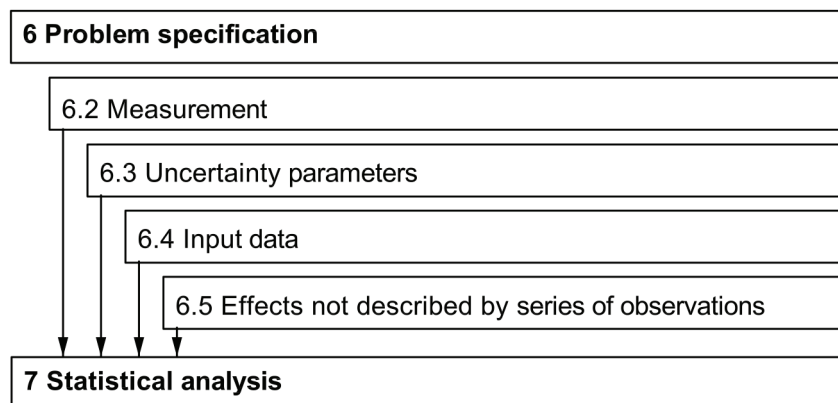


Figure 3 — Elements of problem specification in uncertainty estimation

6.2 Measurement

The measurement shall be specified (at least) in terms of

- measurand,
- method of measurement,
- method model equation $y = f(x_1, \dots, x_K)$, if results of measurement y are calculated from observed or otherwise known input quantities x_i , and
- intended application of the method of measurement.

The measurand shall be specified in such a way that it is expected to exhibit an unknown, but unique, value μ at least for the time period needed to perform a single measurement.

The measurand is the physical quantity to be assigned a numerical value and a unit of measurement by means of the specified measurement. Furthermore, the measurand shall be specified in such a way that it could be subjected, at least in principle, to more than a single measurement. This is more important for the provision of input data for uncertainty estimation than for routine execution of a considered method of measurement. In air quality, the measurand can change value as a function of time and space.

The method of measurement shall be specified completely, e.g. by

- the applicable procedure, e.g. the standard operating procedure (SOP),
- the type of application (e.g. in routine monitoring of stationary source emissions, in routine monitoring of workplace atmospheres, in routine monitoring of ambient air, or as a reference standard in a laboratory),
- the ambient conditions of that application (e.g. variations in ambient conditions), and
- the conditions of control, (e.g. for calibration or drift control).

Often, appropriate descriptions are available as part of the method documentation.

Additional information on the method of measurement can be provided, e.g. on effects causing variations and bias in the considered application.

If a method model equation $y = f(x_1, \dots, x_K)$ is used to obtain results of measurement y in intended use from observed or otherwise known input quantities x_i , its mathematical structure shall be known for evaluation of an indirect approach. For an introductory explanation of the direct and the indirect approach, see [5.4](#).

NOTE 1 In this International Standard, the measurand is understood to be a quantifiable property of an object of measurement. The object of measurement can be, e.g. the gas emitted by a stack of specified cross-section within a specified time period, or the ambient air at a specified sampling location within a defined time interval. The corresponding measurand can be, e.g. the mass (flow) of sulfur dioxide emitted by the specified stack within the specified time period, or the concentration of sulfur dioxide in ambient air at the specified location within the defined time interval.

NOTE 2 The method model equation is sometimes called the "analytical equation" in air quality measurement.

The intended application of the method of measurement shall be specified in such a way that the representativeness of the input data can be assessed properly. This is necessary in order to ensure, that an obtained uncertainty parameter is appropriate to describe results of measurement obtained in the intended application of the method of measurement. In statistical terms, the application of the method of measurement describes the statistical population of possible results of measurement Y to be considered in the uncertainty estimation.

The application of the method of measurement can be specified in different ways, e.g. as follows:

- an application of an individual measuring system under well defined laboratory conditions;
- an application of different measuring systems of the same type operated in a monitoring network by the same laboratory;
- an application of different measuring systems of the same type operated in a wide range of field conditions by different laboratories.

6.3 Uncertainty parameters

The required uncertainty parameter shall be specified. The uncertainty parameter to be provided for the specified population of results of measurement y can be one of the following quantities:

- (combined) standard uncertainty $u(y)$ in units of y ;
- relative standard uncertainty $w(y)$;

- expanded uncertainty $U_p(y)$ on a specified level of coverage p in units of y ;
- relative expanded uncertainty $W_p(y)$ on a specified level of coverage p .

Uncertainty estimation can be simplified considerably, if a common uncertainty parameter is applicable to a specified range of values y of the result of measurement. For more information on uncertainty parameters, see [Clause 9](#).

6.4 Input data

6.4.1 General

At least the following details on input data for uncertainty estimation shall be described:

- the approach used to investigate variation and bias occurring in intended use of the method of measurement;
- the experimental design(s) used to collect the series of observations;
- the series of observations to be evaluated;
- the representativeness of the series of observations provided as input data.

The approach used to investigate variations and bias can be either an indirect approach or a direct approach.

In a direct approach, input data are obtained in a single experimental design that provides information on deviations and bias by comparison with one or more reference values of the measurand.

In an indirect approach, input data are obtained in different experimental designs for the different input quantities x_i of the method model equation $y = f(x_1, \dots, x_K)$ used to calculate the result of measurement y .

[Table 1](#) summarizes the experimental designs A1 to A8 considered in this International Standard. Applicable evaluation methods of Type A for these experimental designs are described in [Annex B](#).

Table 1 — Experimental designs and input data

Type	Experimental design	Typical application	Input data	
			Direct approach	Indirect approach
A1	Simple random sampling	Repeated unbiased observation of the same (unknown) measurand by means of the same measuring system	$y(j)$ with $j = 1$ to N	$x_i(j)$ with $j = 1$ to N
A2	Repeated observation of a reference material by a measuring system	Drift control procedure applied to the measuring system	$y(j)$ with $j = 1$ to N y_R	$x_i(j)$ with $j = 1$ to N $x_{R,i}$
A3	Observation of different reference materials in a calibration procedure	Calibration procedure providing at least 3 repeated observations of each reference materials	$x(j)$ with $j = 1$ to N $y_R(j)$ with $j = 1$ to N	$z(j)$ with $j = 1$ to N $x_R(j)$ with $j = 1$ to N
A4	Observation of different reference materials by identical measuring systems	Method validation before routine application providing N independent observations of different reference materials	$x(j)$ with $j = 1$ to N $y_R(j)$ with $j = 1$ to N	$z(j)$ with $j = 1$ to N $x_R(j)$ with $j = 1$ to N
A5 Case 1	Parallel measurements with a reference method of measurement	Calibration procedure providing N uncorrected outputs in parallel measurements with a reference method of measurement	$x(j)$ with $j = 1$ to N $y_R(j)$ with $j = 1$ to N	$z(j)$ with $j = 1$ to N $x_R(j)$ with $j = 1$ to N
A5 Case 2	Parallel measurements with a reference method of measurement	Verification procedure providing N corrected outputs in parallel measurements with a reference method of measurement	$y(j)$ with $j = 1$ to N $y_R(j)$ with $j = 1$ to N	$x(j)$ with $j = 1$ to N $x_R(j)$ with $j = 1$ to N
A6	Paired measurement of two identical measuring systems	Validation of a reference method of measurement; Validation of a calibrated method of measurement.	$\{y(1, j); y(2, j)\}$ with $j = 1$ to N	$\{x(1, j); x(2, j)\}$ with $j = 1$ to N
A7	Interlaboratory comparison of identical measuring systems	Comparison providing N observations of the same measurand by K laboratories using the same method of measurement	$y(k, j)$ with $j = 1$ to N and $k = 1$ to K	$x(k, j)$ with $j = 1$ to N and $k = 1$ to K
A8	Parallel measurement of identical measuring systems	N parallel measurements with K identical measuring systems	$y(k, j)$ with $j = 1$ to N and $k = 1$ to K	$x(k, j)$ with $j = 1$ to N and $k = 1$ to K

Experimental designs not mentioned in [Table 1](#) may be evaluated as well for uncertainty estimation, if their execution and statistical evaluation is documented in sufficient detail.

The experimental design(s) used to collect input data shall be documented in sufficient detail to assess the representativeness of the input data for the possible results of measurement to be described by the specified uncertainty parameter. The results of assessing the representativeness of the input data shall be documented.

6.4.2 Assessment of representativeness

For the series of observations provided as input data, it shall be assessed whether in the applied data collecting procedure

- the method of measurement was operated in accordance with the same standard operating procedure as in the intended application,
- the ambient conditions covered at least the range of variation expected to occur in the intended application of the method of measurement,
- the conditions of control of the method of measurement were the same as in the intended application,

- d) if appropriate, the reference standards used to correct the method of measurement were of the same quality as those applied in intended use,
- e) all parts of the method of measurement were subjected to an experimental design either separately or pooled providing the considered series of observations, and
- f) if appropriate, operation of the method of measurement by different laboratories was evaluated in an experimental design.

If the statements a) to f) are fulfilled appropriately, the provided series of observations are considered representative for the specified uncertainty estimation. Statement d) applies to methods of measurement requiring correction for systematic effects. Statement f) applies, if the uncertainty parameter shall describe results of measurement (to be) obtained by different laboratories in application of the specified method of measurement.

If one or more of the statements a) to f) are not all fulfilled appropriately, additional input is needed to provide representative input data. Additional input data can be provided either by provision of more appropriate series of observations, or by expert judgement as described in [6.5](#).

6.5 Effects not described by series of observations

If an effect causing variations or bias is not described in a representative way by a series of observations, although it is expected to influence possible results of measurement, this effect shall be described separately, e.g. by an additional deviation δY_j of the result of measurement. The numerical values of such an additional deviation shall be assessed by expert judgement. The basic task of this expert judgement is the provision of an estimate of the maximum range $[\min(\delta Y_j) \leq \delta Y_j \leq \max(\delta Y_j)]$ of the deviation δY_j . This information is needed to provide an estimate $\text{var}(\delta Y_j)$ of the variance of the deviation δY_j . Details on variance estimation based on expert judgement (Type B evaluation) are provided in [8.3](#). A Type B evaluation should only supplement a Type A evaluation.

Instead of estimating the maximum value, $\max(\delta Y_j)$, of a potential deviation δY_j directly, it can sometimes be more convenient to estimate it indirectly by means of [Equation \(1\)](#):

$$\max(\delta Y_j) = c_j \cdot \max(\delta X_j) \quad (1)$$

In the latter case, δX_j designates a potential deviation of the considered influence quantity x_j from a specified reference value, and c_j the sensitivity coefficient of the method of measurement with respect to changes of that influence quantity.

NOTE The sensitivity coefficient c_j can be determined from separate investigation, e.g. within a method validation study.

Typical effects which can sometimes not be described in a representative way by a series of observations are summarized in [Table 2](#) (this list of effects is nonexhaustive).

An additional deviation δY_j may be neglected, if the corresponding variance estimate $\text{var}(\delta Y_j)$ contributes less than 5 % to the variance estimate $\text{var}(Y)$ used in the uncertainty estimation.

Table 2 — Effects which can require separate assessment

No.	Effect	Assessment of possible influence on the result of measurement
1	Sampling efficiency F_{sam} not corrected for by calibration procedure	$\delta Y_{\text{sam}} = y (1 - F_{\text{sam}})$
2	Extraction efficiency F_{ext}	$\delta Y_{\text{ext}} = y (1 - F_{\text{ext}})$
3	Variation of ambient temperature T	$\delta Y_T = c_T \delta T$
4	Variation of ambient pressure P	$\delta Y_P = c_P \delta P$
5	Variation of ambient humidity H	$\delta Y_H = c_H \delta H$
6	Variation of composition of air sampled Y_{INT}	$\delta Y_{\text{INT}} = c_{\text{INT}} Y_{\text{INT}}$
7	Variation of line voltage V	$\delta Y_V = c_V \delta V$

7 Statistical analysis

7.1 Objectives

The objective of statistical analysis in uncertainty estimation is to provide a mathematical rational for calculating an estimate $\text{var}(Y)$ 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 which was executed to obtain the result of measurement y . Based on that variance estimate, the (combined) standard uncertainty $u(y)$ of the result of measurement y is finally calculated by $u(y) = \sqrt{\text{var}(Y)}$.

This International Standard provides guidance to statistical analysis applicable without expertise in statistical modelling of measuring processes. Statistical modelling in the framework of uncertainty estimation is simplified considerably by separate consideration of the indirect and the direct approach. Whereas the recommendations of the GUM are addressed explicitly to the more complex indirect approach, they apply as well to the mathematically much simpler direct approach. In contrast to the indirect approach, a direct approach starts from a single series of observed results of measurement provided as input data.

The appropriate statistical model equation depends on

- the approach used to investigate variations and bias occurring in the method of measurement,
- the experimental design(s) used in that approach,
- the series of observations provided as input data, and
- the representativeness of the input data.

Based on the statistical model equation, an appropriate equation for estimating $\text{var}(Y)$ is obtained by the rule of uncertainty propagation.

If the uncertainty parameter is the coverage probability p of a specified interval $[y - U_p(y); y + U_p(y)]$ about a result of measurement y , statistical analysis can be simplified considerably as described in [9.3](#).

[Table 3](#) emphasizes the differences in the 5-step procedure of uncertainty estimation in the direct and indirect approach.

Table 3 — Elements of uncertainty estimation in direct and indirect approach

Step	Element	Direct approach	Indirect approach
1	Problem specification		
	Experimental design	one experimental design, e.g. of type A1 to A8	more than one experimental design, e.g. of Type A1 to A8
	Input data	one series of observations and reference values of the measurand y See 6.4.	series of observations of input quantities x_i or estimates x_i and $\text{var}(x_i)$ for each input quantity x_i See 6.4.
	Additional deviation	$\min(\delta Y_j) \leq \delta Y_j \leq \max(\delta Y_j)$, if appropriate	$\min(\delta Y_j) \leq \delta Y_j \leq \max(\delta Y_j)$, if appropriate
2	Statistical analysis		
	Method model equation	$y = f(x_1, x_2, \dots)$, if available	$y = f(x_1, x_2, \dots)$
	Statistical model equation	$Y = y + \delta Y$	$Y = f(x_1, x_2, \dots) + \delta Y$
	Variance equation	$\text{var}(Y) = \text{var}(y) + \text{var}(\delta Y)$ See 7.3.	$\text{var}(Y) = c_1^2 \text{var}(x_1) + c_2^2 \text{var}(x_2) + \dots$ $+ 2 c_1 c_2 \text{cov}(x_1, x_2) + \dots$ $+ \text{var}(\delta Y)$ See 7.2.
3	Estimation of variances and covariances		
	Type A	$\text{var}(y) = u^2(y)$ See 8.2 and Annex B.	$\text{var}(x_i) = u^2(x_i)$ See 8.2 and Annex B.
	Type B	$\text{var}(\delta Y) = \dots$ See 8.3.	$\text{var}(\delta Y) = \dots$ See 8.3.
	Covariances	See 8.4.	See 8.4.
4	Evaluation of uncertainty parameters		
	(Combined) standard uncertainty	$u(y) = \sqrt{\text{var}(Y)}$	$u(y) = \sqrt{\text{var}(Y)}$
	Expanded uncertainty	$U_p(y) = k_p(\nu) \cdot u(y)$ See 9.2.	$U_p(y) = k_p(\nu) \cdot u(y)$ See 9.2.
5	Reporting		

Although Y is called the measurand by the GUM, the meaning of Y in the mathematical context of the GUM is that of a random variable describing a "possible result of measurement". The character Y shall not be confused with the unknown but unique value μ of the measurand under observation. The general concept of measurement implies that the measurand exhibits a unique value at least for the time interval described by an individual result of measurement.

7.2 Indirect approach

In an indirect approach, variation and bias are evaluated, in a first step, separately for the input quantities x_i of the method model equation $y = f(x_1, \dots, x_K)$ used to obtain results of measurement y . The following data can be used as input data:

- series of observations of input quantities x_i collected, e.g. in experimental designs of types A1 to A8;

- estimates of x_i and $\text{var}(x_i)$ provided by external sources, such as quantities associated with calibrated measurement standards, certified reference materials, reference data obtained from handbooks and data on reproducibility and trueness.

NOTE The use of external data on reproducibility and trueness for uncertainty estimation is described in ISO/TS 21748[9].

Additional deviations δY_j can be caused by effects not represented by a series of observations. If necessary, these deviations can be assessed by expert judgement and a Type B evaluation.

Under these conditions, an appropriate statistical model equation for uncertainty estimation is provided in generic terms by [Equation \(2\)](#):

$$Y = f(x_1, \dots, x_K) + \sum_{j=1}^M \delta Y_j \quad (2)$$

where

- Y is a possible result of measurement;
- x_i is the input quantity of the method model equation $y = f(x_1, \dots, x_K)$ used to calculate the result of measurement y ;
- δY_j is an additional deviation of result of measurement y not represented by the series of observations of input quantities x_i ;
- K is the number of input quantities of the method model equation;
- M is the number of additional deviations to be assessed by a Type B evaluation.

An additional deviation δY_j shall be taken into account in the statistical model equation given by [Equation \(2\)](#), if the corresponding variance $\text{var}(\delta Y_j)$ makes up at least 5 % of the population variance $\text{var}(Y)$ described in [Equation \(3\)](#). Otherwise, the deviation δY_j may be neglected in the uncertainty estimation.

In a second step, the rule of uncertainty propagation shall be applied to the statistical model equation given by [Equation \(2\)](#). In this way, the variance estimate $\text{var}(Y)$ is obtained from variance (budget) equation as given by [Equation \(3\)](#):

$$\text{var}(Y) = \sum_{i=1}^K c_i^2 \text{var}(x_i) + 2 \sum_{i=1}^K \sum_{j=i+1}^K c_i c_j \text{cov}(x_i, x_j) + \sum_{j=1}^M \text{var}(\delta Y_j) \quad (3)$$

where

- $\text{var}(Y)$ is the estimate of the variance of possible results of measurement Y ;
- c_i is the sensitivity coefficient with respect to variations of input quantity x_i ;
- $\text{var}(x_i)$ is an estimate of the variance of input quantity x_i ;
- $\text{cov}(x_i, x_j)$ is an estimate of covariance between input quantities x_i and x_j ;
- $\text{var}(\delta Y_j)$ is an estimate of the variance of additional deviation δY_j .

In formal terms, the sensitivity coefficient c_i is the partial derivative of the method model function $y = f(x_1, \dots, x_K)$ by [Equation \(4\)](#):

$$c_i = \frac{\partial f(x_1, \dots, x_K)}{\partial x_i} \quad (4)$$

In practical terms, a sensitivity coefficient c_i can be obtained in different ways:

- by application of rules of algebra;
- by a numerical calculation of the derivative;

— as the mean value of the ratio of observed changes $\Delta y(j)$ of the result of measurement divided by the change $\Delta x_i(j)$ causing the observed change $\Delta y(j)$ as given by [Equation \(5\)](#):

$$c_i = \sum_{j=1}^N \frac{[\Delta y(j) / \Delta x_i(j)]}{N} \quad (5)$$

The variance estimates $\text{var}(x_i)$ in [Equation \(3\)](#) shall be evaluated either by a Type A evaluation method appropriate for the experimental design used to obtain the input data or by reference to external sources. Type A methods for the evaluation of the experimental designs A1 to A8 are described in detail in [Annex B](#).

Variance estimates $\text{var}(\delta Y_j)$ of deviations δY_j shall be calculated by a Type B evaluation method described in [8.3](#).

Covariances $\text{cov}(x_i, x_j)$ shall be considered zero if the series of observations provided for the input quantities x_i and x_j were obtained independent of each other in different experimental designs. Otherwise, estimates of covariances $\text{cov}(x_i, x_j)$ shall be calculated by a method described in [8.4](#).

7.3 Direct approach

In a direct approach, variation and bias of results of measurement y are assessed directly in a pooled way in a single experimental design, e.g. of types A1 to A8. Input data are a single series of observations and the corresponding reference values. If necessary, additional deviations δY_j caused by effects not represented by the series of results of measurement are assessed by expert judgement.

Under these conditions, the statistical model equation for uncertainty estimation is given by [Equation \(6\)](#):

$$Y = y + \sum_{j=1}^M \delta Y_j \quad (6)$$

where

Y	is a possible result of measurement;
y	is a result of measurement provided as input data (see 6.4);
δY_j	is an additional deviation of result of measurement y not represented by the series of results of measurement;
M	is the number of additional deviations to be assessed by a Type B evaluation.

An additional deviation δY_j shall be taken into account in the statistical model equation given by [Equation \(6\)](#), if the corresponding variance $\text{var}(\delta Y_j)$ makes up at least 5 % of the estimate $\text{var}(Y)$ of the population variance described in [Equation \(7\)](#). Otherwise, the deviation δY_j may be neglected in uncertainty estimation.

The rule of uncertainty propagation shall be applied to the statistical model equation given by [Equation \(6\)](#). In this way, the variance estimate $\text{var}(Y)$ is obtained from the variance (budget) equation as given by [Equation \(7\)](#):

$$\text{var}(Y) = \text{var}(y) + \sum_{j=1}^M \text{var}(\delta Y_j) \quad (7)$$