
Uncertainty of measurement — Part 6: Developing and using measurement models

Incertitude de mesure —

Partie 6: Élaboration et utilisation de modèles de mesure





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This document was prepared by Working Group 1 of the Joint Committee for Guides in Metrology (as JCGM GUM-6:2020), and was adopted by the national bodies of ISO and IEC.

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Guide to the expression of uncertainty in measurement — Part 6: Developing and using measurement models

Guide pour l'expression de l'incertitude de mesure — Partie 6:
Élaboration et utilisation des modèles de mesure

JCGM GUM-6:2020

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Foreword

In 1997 a Joint Committee for Guides in Metrology (JCGM), chaired by the Director of the Bureau International des Poids et Mesures (BIPM), was created by the seven international organizations that had originally in 1993 prepared the ‘Guide to the expression of uncertainty in measurement’ and the ‘International vocabulary of basic and general terms in metrology’. The JCGM assumed responsibility for these two documents from the ISO Technical Advisory Group 4 (TAG4).

The Joint Committee is formed by the BIPM with the International Electrotechnical Commission (IEC), the International Federation of Clinical Chemistry and Laboratory Medicine (IFCC), the International Laboratory Accreditation Cooperation (ILAC), the International Organization for Standardization (ISO), the International Union of Pure and Applied Chemistry (IUPAC), the International Union of Pure and Applied Physics (IUPAP), and the International Organization of Legal Metrology (OIML).

JCGM has two Working Groups. Working Group 1, ‘Expression of uncertainty in measurement’, has the task to promote the use of the ‘Guide to the expression of uncertainty in measurement’ and to prepare documents for its broad application. Working Group 2, ‘Working Group on International vocabulary of basic and general terms in metrology’, has the task to revise and promote the use of the ‘International vocabulary of basic and general terms in metrology’ (the ‘VIM’).

In 2008 the JCGM made available a slightly revised version (mainly correcting minor errors) of the ‘Guide to the expression of uncertainty in measurement’, labelling the document ‘JCGM 100:2008’. In 2017 the JCGM rebranded the documents in its portfolio that have been produced by Working Group 1 or are to be developed by that Group: the whole suite of documents became known as the ‘Guide to the expression of uncertainty in measurement’ or ‘GUM’. This document, previously known as JCGM 103, Supplement 3 to the GUM, is the first to be published as a part of that portfolio, and is entitled and numbered accordingly.

The present guide is concerned with the development and use of measurement models, and supports the documents in the entire suite of JCGM documents concerned with uncertainty in measurement. The guide has been prepared by Working Group 1 of the JCGM, and has benefited from detailed reviews undertaken by member organizations of the JCGM and National Metrology Institutes.

Introduction

A measurement model constitutes a relationship between the output quantities or measurands (the quantities intended to be measured) and the input quantities known to be involved in the measurement. There are several reasons for modelling a measurement. Models assist in developing a quantitative understanding of the measurement and in improving the measurement. A model enables values of the output quantities to be obtained given the values of the input quantities. Additionally, a model not only allows propagation of uncertainty from the input quantities to the output quantities; it also provides an understanding of the principal contributions to uncertainty. This document is accordingly concerned with the development of a measurement model and the practical use of the model.

One of the purposes of measurement is to assist in making decisions. The reliability of these decisions and the related risks depend on the values obtained for the output quantities and the associated uncertainties. In turn, these decisions depend on a suitable measurement model and the quality of information about the input quantities.

Although the development of a measurement model crucially depends on the nature of the measurement, some generic guidance on aspects of modelling is possible. A measurement model might be a straightforward mathematical relationship, such as the ideal gas law, or, at the other extreme, involve a sophisticated numerical algorithm for its evaluation, such as the detection of peaks in a signal and the determination of peak parameters.

A measurement model may take various forms: theoretical, empirical or hybrid (part-theoretical, part-empirical). It might have a single output quantity or more than one output quantity. The output quantity may or may not be expressed directly in terms of the input quantities. The quantities in the measurement model may be real-valued or complex-valued. Measurement models may be nested or multi-stage, in the sense that input quantities in one stage are output quantities from a previous stage, as occurs, for instance, in the dissemination of measurement standards or in calibration. Measurement models might describe time series of observations, including drift, and dynamic measurement. A measurement model may also take the form of a statistical model. In this document the concept ‘measurement model’ is intended in this broader meaning.

In developing or using a measurement model there are important choices to be made. The selection of a model that is adequate or fit for purpose is a key issue. Particularly for empirical models, there is choice of representation (or parametrization) of the families of functions concerned (polynomials, polynomial splines or rational functions, etc.). Certain choices can be far superior to others in their numerical behaviour when the model is implemented on a computer. The uncertainty arising from the choice of model is a necessary consideration.

In many disciplines, a basic measurement model requires extension to incorporate effects such as temperature corrections arising from the measurement to enable values for output quantities and the associated uncertainties to be obtained reliably.

Following the introduction in 1993 of the Guide to the expression of uncertainty in measurement, or GUM (also known as JCGM 100:2008), the practice of uncertainty evaluation has broadened to use a wider variety of models and methods. To reflect this, this Guide includes an introduction to statistical models for measurement modelling (clause 11) and additional guidance on modelling random variation in Annex C.

Guide to the expression of uncertainty in measurement — Part 6: Developing and using measurement models

1 Scope

This document provides guidance on developing and using a measurement model and also covers the assessment of the adequacy of a measurement model. The document is of particular interest to developers of measurement procedures, working instructions and documentary standards. The model describes the relationship between the output quantity (the measurand) and the input quantities known to be involved in the measurement. The model is used to obtain a value for the measurand and an associated uncertainty. Measurement models are also used in, for example, design studies, simulation of processes, and in engineering, research and development.

This document explains how to accommodate in a measurement model the quantities involved. These quantities relate i) to the phenomenon or phenomena on which the measurement is based, that is, the measurement principle, ii) to effects arising in the specific measurement, and iii) to the interaction with the artefact or sample subject to measurement.

The guidance provided is organised in accordance with a work flow that could be contemplated when developing a measurement model from the beginning. This work flow starts with the specification of the measurand (clause 6). Then the measurement principle is modelled (clause 7) and an appropriate form of the model is chosen (clause 8). The basic model thus obtained is extended by identifying (clause 9) and adding (clause 10) effects arising from the measurement and the artefact or sample subject to measurement. Guidance on assessing the adequacy of the resulting measurement model is given in clause 12. The distinction between the basic model and the (complete) measurement model in the work flow should be helpful to those readers who already have a substantial part of the measurement model in place, but would like to verify that it contains all effects arising from the measurement so that it is fit for purpose.

Guidance on the assignment of probability distributions to the quantities appearing in the measurement model is given in JCGM 100:2008 and JCGM 101:2008. In clause 11, this guidance is supplemented by describing how statistical models can be developed and used for this purpose.

When using a measurement model, numerical problems can arise including computational effects such as rounding and numerical overflow. It is demonstrated how such problems can often be alleviated by expressing a model differently so that it performs well in calculations. It is also shown how a reformulation of the model can sometimes be used to eliminate some correlation effects among the input quantities when such dependencies exist.

Examples from a number of metrology disciplines illustrate the guidance provided in this document.

2 Normative references

The following documents are referred to in the text in such a way that some or all of their content constitutes requirements 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.

BIPM, IEC, IFCC, ILAC, ISO, IUPAC, IUPAP, and OIML. Evaluation of measurement data — Guide to the expression of uncertainty in measurement. Joint Committee for Guides in Metrology, JCGM 100:2008.

BIPM, IEC, IFCC, ILAC, ISO, IUPAC, IUPAP, and OIML. Evaluation of measurement data — Supplement 1 to the ‘Guide to the expression of uncertainty in measurement’ — Propagation of distributions using a Monte Carlo method. Joint Committee for Guides in Metrology, JCGM 101:2008.

BIPM, IEC, IFCC, ILAC, ISO, IUPAC, IUPAP, and OIML. Evaluation of measurement data — Supplement 2 to the ‘Guide to the expression of uncertainty in measurement’ — Extension to any number of output quantities. Joint Committee for Guides in Metrology, JCGM 102:2011.

BIPM, IEC, IFCC, ILAC, ISO, IUPAC, IUPAP, and OIML. International vocabulary of metrology — Basic and general concepts and associated terms. Joint Committee for Guides in Metrology, JCGM 200:2012.

3 Terms and definitions

The terms and definitions of JCGM 100:2008, JCGM 101:2008, JCGM 102:2011 and JCGM 200:2012 apply.

ISO, IEC and IUPAC maintain terminological databases for use in standardization at the following addresses:

- IEC Electropedia: available at <http://www.electropedia.org>
- ISO Online Browsing Platform: available at <http://www.iso.org/obp>
- IUPAC Gold Book: available at <http://www.goldbook.iupac.org>

4 Conventions and notation

4.1 The conventions and notation in JCGM 100:2008, JCGM 101:2008 and JCGM 102:2011 are adopted. Principal symbols used throughout the document are explained in annex A. Other symbols and those appearing in examples are explained at first occurrence.

4.2 Most examples in this document contain numerical values rounded to a number of decimal digits appropriate to the application. Because of rounding there are often numerical inconsistencies among the values presented. An instance is the correlation coefficient of -0.817 in the example in 8.1.6. It is obtained from the *computer-held values* of two

standard uncertainties and a covariance. If it were computed from the three presented values (three significant decimal digits), its value correct to three decimal digits would be -0.822 .

4.3 Links to numbered subclauses are indicated by underlining.

5 Basic principles

5.1 A *measurand* (see JCGM 200:2012, 2.3) is in many cases not measured directly, but is indirectly determined from other *quantities* (see JCGM 200:2012, 1.1) to which it is related by a *measurement model* (see JCGM 200:2012, 2.48) such as formula (1) in 5.2. The measurement model is a mathematical expression or a set of such expressions (see JCGM 100:2008, 4.1.2), comprising all the quantities known to be involved in a measurement. It enables a value (see JCGM 200:2012, 1.19) of the measurand to be provided and an associated standard uncertainty to be evaluated. The measurement model may be specified wholly or partly in the form of an algorithm. The quantities to which the measurand is related constitute the *input quantities* (see JCGM 200:2012, 2.50) in the measurement model. The measurand constitutes the *output quantity* (see JCGM 200:2012, 2.51).

5.2 Many measurements are modelled by a real functional relationship f between N real-valued input quantities $X_1, \dots, X_N$ and a single real-valued output quantity (or measurand) Y in the form

$$Y = f(X_1, \dots, X_N). \quad (1)$$

This simple form is called a real explicit univariate measurement model; real since all quantities involved take real (rather than complex) values, explicit because a value for Y can be computed directly given values of $X_1, \dots, X_N$, and univariate since Y is a single, scalar quantity. However, it does not apply for all measurements. A measurement model can be complex, involving *complex-valued quantities* (see JCGM 102:2011, 3.2). It can be *implicit* where a value for Y cannot be determined directly given values of $X_1, \dots, X_N$ (see 13.5). The measurement model can be *multivariate* where there is more than one measurand, denoted by $Y_1, \dots, Y_m$; for further information, see 13.4 and JCGM 102:2011.

EXAMPLE *Volume of a cylinder*

The volume of a cylinder is given by the measurement model

$$V = \frac{\pi}{4} L d^2$$

in which cylinder length L and diameter d are the $N = 2$ input quantities, corresponding to X_1 and X_2 , and an output quantity V corresponding to Y .

5.3 The process of building a measurement model can be subdivided into the following steps, each step being described in the indicated clause:

- a) Select and specify the measurand (see clause 6).

- b) Model the measurement principle, thus providing a basic model for this purpose (see clause 7), choosing an appropriate mathematical form (see clauses 8 and 11).
- c) Identify effects involved in the measurement (see clause 9).
- d) Extend the basic model as necessary to include terms accounting for these effects (see clauses 10 and 11).
- e) Assess the resulting measurement model for adequacy (see clause 12).

In any one instance, a number of passes through the process may be required, especially following step c). It may be more efficient or effective to take the steps as listed in a different order.

5.4 The manner in which a measurement model is used to obtain a value for the measurand (or values for the measurands) and evaluate the associated standard uncertainty (or covariance matrix) depends on its mathematical form (see clause 13). JCGM 100:2008 mainly considers explicit univariate models and applies the law of propagation of uncertainty (LPU). JCGM 102:2011 gives guidance on the use of generalizations of LPU for multivariate models and implicit models. For non-linear models, the use of the Monte Carlo method of JCGM 101:2008 (univariate measurement models) and JCGM 102:2011 (multivariate models) is often more appropriate (see clause 13).

5.5 The measurement model is a mathematical relationship among quantities, and as such it is subject to the rules of quantity calculus [20]. The same symbols used for the quantities are also used for the corresponding *random variables* (see JCGM 100:2008, C.2.2), whose *probability distributions* (see JCGM 101:2008, 3.1) describe the available knowledge about the quantities. Therefore, the measurement model can also be considered to be a model involving random variables, subject to the rules of mathematical statistics. The law of propagation of uncertainty as described in JCGM 100:2008, 5.1 and 5.2 uses a simple property of the transformation of *random variables* when only expectations and variances (and, perhaps, covariances) are used, rather than the whole distributions.

EXAMPLE *Mass of a spherical weight*

The mass of a weight that has been machined in the form of a sphere from a block of material is given by

$$m = \frac{\pi}{6} d^3 \rho, \quad (2)$$

where d is the diameter of the weight and ρ is the density of the material.

Expression (2) is a simple, well-known physical model that is idealized, applying to a perfect sphere and relating the output quantity mass to the input quantities diameter and density. At the same time, d and ρ can be considered as random variables describing the available information on the corresponding physical quantities obtained, for instance, from a dimensional measurement made with a vernier caliper and from a table of reference data, respectively. Thus, expression (2) also describes how to transform this information about the input physical quantities to the mass m of the weight (the measurand).

5.6 When building a measurement model that is fit for purpose, all effects known to affect the measurement result should be considered. The omission of a contribution can lead to an unrealistically small uncertainty associated with a value of the measurand [156], and even to a wrong value of the measurand.

Considerations when building a measurement model are given in 9.3. Also see JCGM 100:2008, 3.4.

5.7 The fitness for purpose of a measurement model can encompass considerations made before measurement. Such aspects include the measurement capability [85] (see JCGM 200, 2.6) in the case of a laboratory routinely performing calibrations. Fitness for purpose can also encompass the cost of measurement at a given level of uncertainty compared with the consequent costs of incorrect decisions of conformity (see also JCGM 106:2012 [21]). The measurand, which in the terminology of conformity assessment is a 'quality characteristic of the entity', can be, as in statistics, either

- a measure of 'location', for instance, a quantity relating to an entity such as the mass of a single object, an error in mass (deviation from a nominal value), or an average mass of a batch of objects, or
- a measure of 'dispersion', for instance, the standard deviation in mass amongst a batch of objects in a manufacturing process.

5.8 When developing a measurement model, the ranges of possible values of the input quantities and output quantities should be considered. The model should be capable of providing credible estimates and associated uncertainties for all output quantities over the required ranges of the input quantities, which should be specified as appropriate. The measurement model should only be used within the ranges of all quantities for which it has been developed and assessed for adequacy. See 13.2.

5.9 One aspect of specifying the domain of validity of the measurement model (see also 5.8) is to identify any restrictions on the domains of the quantities involved in the measurement model. Some quantities are necessarily positive (or at least non-negative). Some quantities might have lower and upper limits. There can be interrelationships between two or more quantities that need to be included in the measurement model.

EXAMPLE *Quantities having restrictions*

- Positive quantities, for instance, mass and volume.
- Quantity with limits, for instance, a mass fraction can only take values between zero and one.
- Quantities having interrelationships, for instance, the relative proportions (fractions) of all components (hydrocarbons and other molecules) of a natural gas sum to a constant.

Such quantities can sometimes be re-expressed by applying transformations. For instance, denoting by θ a new real quantity that is unconstrained:

- a quantity q is positive if re-expressed as $q = \theta^2$,
- a quantity q lies between a and b if re-expressed as $q = a + (b - a) \sin^2 \theta$, and
- quantities q_1 and q_2 sum to unity by the transformation $q_1 = \sin^2 \theta$, $q_2 = \cos^2 \theta$.

6 Specifying the measurand

6.1 The choice of the measurand depends on the purpose of the measurement and may take account of the *target measurement uncertainty* (see JCGM 200, 2.34). Other processes and measurands are possible and the appropriate choice depends on the application of the measurement result.

NOTE Some measurands may be time-dependent such as in 10.6 and annex B.

EXAMPLE *Diameter of a cylindrical component*

In dimensional metrology, the diameter of a component of cylindrical form is obtained from knowledge of the profile of a right section of the component. If the component is a cylindrical piston, which is required to fit inside the cylinder of a piston-cylinder assembly, the measurand is the diameter of the minimum circumscribing circle (MCC) for the profile. Figure 1 (left) gives the MCC for a lobed profile.

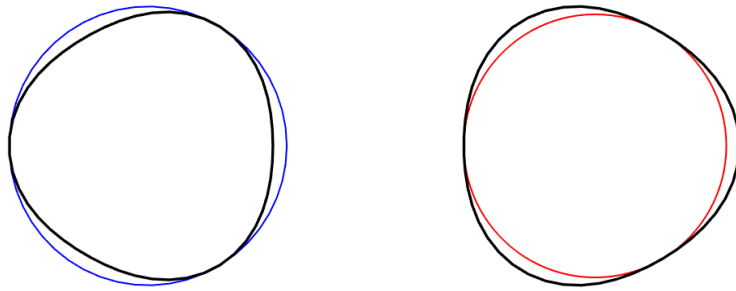


Figure 1: Minimum circumscribed circle (left, blue) and maximum inscribed circle (right, red), described by thin lines, for lobed profiles indicated by thick curved lines

If the component is a cylinder, which is required to contain a cylindrical piston in a piston-cylinder assembly, the measurand is the diameter of the maximum inscribed circle (MIC) for the profile. Figure 1 (right) gives the MIC for a lobed profile.

The profiles exhibit lobing due to the machining process used to produce the corresponding parts. For further information see reference [68] (Calibration Guide 6). Reference [6] describes how to determine MCC and MIC by expressing the problems as optimization problems with linear constraints, a 'standard form' for solution.

6.2 Taking account of any given target measurement uncertainty, the measurand should be specified sufficiently well so that its value is unique for all practical purposes related to the measurement. Regulations, legislation or contracts can contain stipulations concerning the measurand, and often these documents specify a measurand to the relevant extent, for instance, by reference to an international standard (such as ISO or IEC) or OIML recommendation. In general, an adequate specification of the measurand would often involve location in space and time of the measurement, or specification of reference conditions of, for example, temperature and pressure.

EXAMPLE *Length of a gauge block* (also see example in 13.3)

The (central) length of a gauge block is defined as the perpendicular distance between the central point of one end face and a plane in contact with the opposite end face, when the gauge block is at 20 °C.

6.3 In material testing, the measurand is often some property of an entire bulk of material under consideration. The measurement result to be obtained is required to be valid for the bulk (population) from which the sample is taken for measurement or testing. In such cases the measured value can be obtained through a process of sampling and measurement. Aspects such as the uncertainty arising from sampling, or also sample processing, are often

part of the specification of the measurand in these circumstances. Often these aspects are covered in a sampling plan (see, for instance, ISO/IEC 17025 [100]). Also see [6.1](#).

EXAMPLE 1 *Rockwell C hardness*

Rockwell C hardness is defined as hardness value, measured in accordance with ISO 6508, obtained using a diamond cone indenter and a force of 1 471 N [9, 95]. Possible ways to specify the measurand relating to Rockwell C hardness of a material can relate to a specified point on the material (or on a sample from it) at a specified time, and mean Rockwell C hardness of the material. The latter is typically obtained as the average over designated points (in the material itself or in the sample) at a specified time. The specification of the measurand as 'Rockwell C hardness of the material' would only be adequate if the sample (and the material) were substantially homogeneous and stable for the intended use of the material.

EXAMPLE 2 *Emission monitoring*

Two possible measurands relating to a component in an effluent are its mass concentration at the time of sampling and its total mass over a calendar year. In the fields related to power production, emissions are often also qualified in terms of mass emitted per unit of energy produced.

EXAMPLE 3 *Biological material measurement*

For a consignment of biological material subject to measurement, the measurand might relate to a particular sample of the material, a set of samples, the method used to make the measurement, the laboratory performing the measurement, or a set of laboratories involved in making the measurement.

6.4 The specification of a measurand often requires describing the conditions for which the measurement result is valid.

EXAMPLE 1 *Catalytic activity*

The catalytic activity of an enzyme depends on the pH, temperature and other conditions. A complete specification of the measurand therefore requires these conditions to be specified.

EXAMPLE 2 *Calorific value of natural gas*

The calorific value (or, more correctly, the enthalpy of combustion) of natural gas is a function of temperature and pressure. When specifying the measurand, the relevant temperature and pressure are part of that specification. For example, reference conditions could be 288.15 K and 101.325 kPa [87]. Often there are contractually agreed reference conditions specified.

6.5 The measurement procedure should, as appropriate, address how the result is converted from the conditions of measurement to the conditions for which it is reported.

EXAMPLE 1 *Length of a gauge block* (also see example in [13.3](#))

The standard reference temperature for dimensional metrology is 20 °C [86]. This standard reference temperature is exact, so that the laboratory temperature, even in the most sophisticated systems, can only approximate it. Consequently, the measurement model for the length of the gauge block in the example in [6.2](#) contains a correction to that length based on i) the temperature difference between the reference temperature and the laboratory temperature (for example, 23 °C), and ii) the average coefficient of linear expansion in that range. Even when the *indicated* laboratory temperature is 20 °C and the value of the correction would be equal to zero, there would still be a non-zero associated uncertainty.

EXAMPLE 2 *Natural gas volume*

Natural gas volume is measured at the metering pressure and temperature of the gas in the transfer line. The volume is reported at reference conditions for pressure and temperature, which are agreed

between the contracting parties. The conversion of the natural gas volume at metering to reference conditions involves, among others, the compressibility factor of the natural gas at metering and reference conditions. The conversion is part of the measurement model.

6.6 In general, the same measurand can be represented by different models, depending primarily on the measurement principle chosen for its determination. Even within the same measurement principle, different models would result from different practical implementations of that principle, from the level of detail in the description of the measurement and the specific mathematical representation chosen among many that are often possible.

EXAMPLE SI value of the Boltzmann constant

The SI value of the Boltzmann constant [125] was obtained from three different measurement principles, to which correspond as many measurement methods: acoustic gas thermometry, dielectric constant gas thermometry and Johnson noise thermometry. A specific measurement model holds for each of these methods. In addition, differences exist even among the models of those laboratories using the same method, due to different practical implementations of the method, and perhaps to the level of detail in identifying effects.

6.7 Ultimately, the measurement model describes the realization of the measurand according to the knowledge of those involved in the measurement. The description may not fully represent the measurand because some unrecognized effects were not included. As a consequence, the uncertainty associated with the estimate of the measurand will not contain the contributions from those effects.

EXAMPLE Mass comparison

In modern mass comparators, the mass m_w of a standard weight W is determined (say, in vacuum) by comparing the forces $F_w = g_w m_w$ and $F_r = g_r m_r$ exerted on the comparator pan by W and by a reference mass standard R, subjected to local accelerations due to gravity g_w and g_r , respectively. The pan is held at a constant level by a servo mechanism. In most applications, it can safely be assumed that $g_w = g_r = g$, so that the model takes the simple form $m_w = m_r - \Delta m$, where Δm is the comparator indication and g has been dropped.

The assumption $g_w = g_r = g$ is correct when the centres of gravity of the two standards during weighings lie at the same elevation, and can anyway be adequate depending on the target uncertainty. If this is not the case, the model may need to be extended, usually with a correction (a further input quantity to the measurement model) to the mass m_r of the reference standard, having the form

$$m_r \frac{\Delta g}{g} \frac{1}{\Delta h} (h_r - h_w),$$

where $\Delta g / (g \Delta h) \approx -2.4 \times 10^{-7} \text{ m}^{-1}$ is the relative vertical gradient of the local acceleration due to gravity and $h_r - h_w$ is the difference in elevation between the centres of gravity of the standards being compared. Whereas the uncertainty associated with the correction is normally negligible, the correction itself can be significant. This is the case in the comparisons at the highest level of standards made of materials having very different densities (and consequently different sizes and sometimes shapes), such as silicon, stainless steel and platinum-iridium standards. Neglecting to include such a correction in the model would imply an incomplete description of the measurand, resulting in an error with respect to a correctly specified measurand. The error amounts to about $-3 \mu\text{g}$ when comparing a stainless steel standard with a platinum-iridium prototype. This value is of the same order of magnitude of the standard uncertainty associated with the estimate of the measurand.

7 Modelling the measurement principle

7.1 General

The measurement principle (see JCGM 200, 2.4) enables a basic model, often based on a scientific law, or combination of such laws, to be established. A set of input quantities, namely, those quantities appearing in the laws underlying the measurement, follows from the measurement principle.

NOTE In many standardized test methods, as published by ISO and IEC for instance, the measurement principle is already described in the form of one or more mathematical formulæ.

EXAMPLE *Simple theoretical model of mass measurement*

The mass m of a weight is measured with a spring balance. The relationship between the restoring force F exerted by the spring and m at equilibrium is $F = mg$, where g is the acceleration due to gravity. Hooke's law relating F to the extension X of the spring and the spring constant k is $F = kX$. Thus, a theoretical measurement model relating mass to extension, spring constant and acceleration due to gravity is

$$m = \frac{k}{g}X.$$

Available knowledge about X , k and g enables knowledge about m to be inferred. Since Hooke's law only applies when the extension is sufficiently small, this measurement model should only be used within this limit. The largest mass, for a given k , for which the restoring force is proportional to the extension of the spring defines the domain of validity of the measurement model (see 5.8).

7.2 Theoretical, empirical and hybrid measurement models

7.2.1 A theoretical measurement model is based on scientific theory that describes how the output quantities in the measurement model relate to the input quantities.

EXAMPLE 1 *SI value of the Avogadro constant*

The Avogadro constant N_A is the universal proportionality constant relating in any sample the number $N(X)$ of entities X and the corresponding amount of substance $n(X)$,

$$N_A = \frac{N(X)}{n(X)}.$$

In the SI, the Avogadro constant has the exact value $N_A = 6.022\,140\,76 \times 10^{23} \text{ mol}^{-1}$ [125]. One of the most accurate methods that was used to determine this value is the X-ray crystal density (XRCD) method [110]. In XRCD, the sample is a near-perfect sphere of mono-crystalline, isotopically enriched silicon (99.99% ^{28}Si). The number of silicon atoms in this sample is $N(\text{Si}) = 8V/a_0^3$, V and a_0^3 being respectively the volumes of the sphere and of the unit atomic cell, containing 8 atoms. The amount of silicon is $n(\text{Si}) = m/M$, where m and M are the mass of the sphere and the molar mass of silicon. Therefore the definition of the Avogadro constant may be written as

$$N_A = \frac{N(\text{Si})}{n(\text{Si})} = \frac{8V}{a_0^3} \frac{M}{m},$$

which is the basic model describing the measurement principle for the XRCD experiment.

EXAMPLE 2 *Pressure generated by a pressure balance* (continued in 8.1.4)

The pressure p generated by a pressure balance is given implicitly by the measurement model

$$p = \frac{m \left(1 - \frac{\rho_a}{\rho_m} \right) g}{A_0 (1 + \lambda p) [1 + \alpha (t - t_{\text{ref}})]}, \quad (3)$$

where m is the total applied mass, ρ_a and ρ_m are respectively the mass densities of air and the applied mass, g is the local acceleration due to gravity, A_0 is the effective area of the piston-cylinder assembly at zero pressure and a reference temperature, λ is the distortion coefficient of the piston-cylinder assembly, α is the temperature coefficient, t is Celsius temperature, and t_{ref} is a reference temperature, 20 °C, say [113]. There are eight input quantities $A_0, \lambda, \alpha, t, m, \rho_a, \rho_m, g$ and a single output quantity p .

7.2.2 Sometimes the measurement principle can only be formulated in terms of an empirical model. For such a model, the measurand would often be expressed in terms of mathematical functions such as polynomials, polynomial splines or rational functions, all of which have adjustable parameters. These models are often expressed as statistical models (see clause 11). Estimates of the parameters of these functions can be provided by reference tables (for instance, see example 2 in 8.3.3) or obtained by data analysis (least-squares regression, say), together with the associated standard uncertainties and covariances.

EXAMPLE *Industrial platinum resistance thermometer*

Platinum resistance thermometers of nominal resistance 100 Ω , also called Pt100 sensors, are used in industry for accurate measurement of temperature. The resistance R of the sensor as a function of Celsius temperature t is modelled over the interval $[-200\text{ °C}, 800\text{ °C}]$ using the empirical Callendar-Van Dusen equation [51]

$$R(t) = \begin{cases} R_0 [1 + At + Bt^2 + Ct^3(t - t_{\text{ref}})], & -200\text{ °C} \leq t < 0\text{ °C}, \\ R_0 (1 + At + Bt^2), & 0\text{ °C} \leq t \leq 800\text{ °C}, \end{cases} \quad (4)$$

where $t_{\text{ref}} = 100\text{ °C}$, being a reference value, has no associated uncertainty, and R_0, A, B and C are determined by calibration. Typical values are $\hat{R}_0 = 100\ \Omega$, $\hat{A} = 3.9 \times 10^{-3}\text{ °C}^{-1}$, $\hat{B} = -6 \times 10^{-7}\text{ °C}^{-2}$, and $\hat{C} = -4 \times 10^{-12}\text{ °C}^{-4}$.

Expression (4) is then used to provide values of the measurand t given values for the input quantities R_0, A, B, C and R and is thus an implicit measurement model (see 13.5).

7.2.3 Most measurement models are hybrid, that is, they combine aspects of theoretical and empirical models. Even if the complete measurement principle is based on scientific theory, there are often quantities involved in the measurement that need to be included in the measurement model and are modelled empirically (also see clauses 9 and 10).

EXAMPLE *Spectral irradiance of a lamp: hybrid model*

A tungsten filament lamp source emits light when its filament is heated by an electric current. The primary physics behind this process is that of a hot source and to first order the lamp acts in a manner similar to a blackbody source. The spectral radiance of a blackbody source can be modelled using the Planck function

$$L(\lambda, T) = \frac{c_{1,L}}{\lambda^5 \{ \exp[c_2/(\lambda T)] - 1 \}},$$

where λ denotes wavelength, T the blackbody temperature and the coefficients $c_{1,L}$ and c_2 can be expressed in terms of fundamental physical constants [5].

Since lamps are not ideal blackbody sources, the emissivity of the tungsten filament and the transmittance of the bulb should be considered. For tungsten filament lamps used as standards, their spectral irradiance varies smoothly with wavelength and can be modelled by the product of a polynomial in λ and a Planck function. (Spectral irradiance is related to radiance by a constant factor depending on geometry.) Such a function is known as a Planck-polynomial function [41, 79]:

$$F(\lambda, T, a_1, \dots, a_p) = L(\lambda, T)G_p(\lambda, a_1, \dots, a_p). \quad (5)$$

The correction factor $G_p(\lambda, a_1, \dots, a_p)$ is an empirical polynomial function of order p in λ with adjustable parameters $a_1, \dots, a_p$. These parameters are estimated by fitting model (5) to suitable data using regression analysis.

7.3 Differential equation models

7.3.1 Many theoretical models used in science, engineering and medicine specify the rates at which some quantities vary as functions of time and other quantities, and are formulated as differential equations [152]. In some cases, the differential equation is only used as a foundation to develop simpler models.

EXAMPLE Vapour pressure at vapour-liquid equilibrium

The vapour pressure equations used in example 1 in 8.1.4 are solutions of the Clausius-Clapeyron relation, which is a differential equation,

$$\frac{dp}{dT} = \frac{\Delta s}{\Delta v}, \quad (6)$$

where p denotes the pressure, the measurand, and T the thermodynamic temperature of the vapour-liquid equilibrium, and Δs and Δv the differences in specific entropy and molar volume, respectively, between the two phases [11].

7.3.2 In measurement models that involve differential equations, the measurand is typically a function of coefficients in these equations. These coefficients are estimated based on empirical data, usually by application of a statistical method (see also clause 11). The equations are solved in the process, often a number of times, usually employing numerical methods, and typically a Monte Carlo method, similar to that described in JCGM 101:2008, is used for uncertainty evaluation [31, 55, 137, 153].

EXAMPLE SIR model for influenza infection

The numbers of cases reported once per week during an influenza epidemic in an isolated village with $n = 327$ inhabitants, during the first 11 weeks of their influenza season were (1, 0), (8, 0), (15, 4), (22, 26), (29, 61), (36, 67), (43, 42), (50, 40), (57, 23), (64, 13), (71, 5). The first element of each pair is the day since the beginning of the season, and the second is the number of people known to have influenza on that day. For instance, the first pair means that on day 1 there were 0 cases, and the last pair means that on day 71 there were 5 cases.

The simple SIR model [102] for the spread of infectious diseases through a population does not contemplate births or deaths occurring during the course of the epidemic. It regards the population as partitioned into three subsets at each time instant t : those that are susceptible to the infection but not yet sick, $S(t)$, those that are infected, $I(t)$, and those that have already recovered from

the infection and are no longer contagious, $R(t)$. Their numbers add up to the population total, $S(t) + I(t) + R(t) = n$, and satisfy three simultaneous differential equations:

$$\frac{dS}{dt} = -\beta I(t)S(t)/n, \quad \frac{dI}{dt} = \beta I(t)S(t)/n - \gamma I(t), \quad \frac{dR}{dt} = \gamma I(t), \quad (7)$$

for some specified non-negative initial values $S(0)$, $I(0)$ and $R(0)$. The model parameters are such that $1/\gamma$ is the typical duration of the infection in an infected person and the parameter of interest is the average number of individuals directly infected by an infectious person in a population where everyone is susceptible, known as the *basic reproduction number* $R_0 = \beta/\gamma$. The model is completed by assuming that the actual number of cases at time t is a random variable $N(t)$ with a Poisson distribution with mean $I(t)$.

Computing the maximum-likelihood estimates [133] of β , γ and $S(0)$ involves finding the values of these parameters that maximize a product of Poisson probability densities (one for each of the 11 days with a reported number of cases), whose means are $I(1)$, $I(8)$, $\dots$, $I(71)$. Since equations (7) cannot be solved analytically, each time the likelihood function needs to be evaluated in the course of the maximization process, these differential equations have to be solved, also numerically. The resulting parameter estimates are $\hat{\beta} = 0.34 \text{ d}^{-1}$ and $\hat{\gamma} = 0.14 \text{ d}^{-1}$, and hence $\hat{R}_0 = 2.4$. Figure 2 (left) depicts the data, the model as fitted to the observations, and the fitted values on the same days when the numbers of influenza cases were observed.

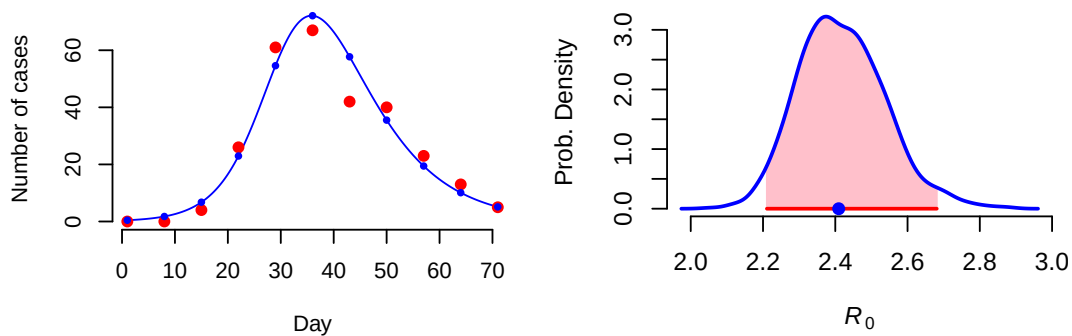


Figure 2: Observed numbers of cases (large, red dots), calibrated model $\hat{I}$ (solid blue curve), and expected numbers of cases (small blue dots) corresponding to the observed numbers of cases and (right) probability density of R_0 based on a sample of size 1 000 drawn from its distribution by a Monte Carlo method, with the blue dot marking the maximum-likelihood estimate, the shaded area comprising 95 % of the area under the curve, and the thick, horizontal red line segment representing a 95 % coverage interval for the reproduction number

The uncertainty associated with the basic reproduction number was evaluated by application of the parametric bootstrap [53], a Monte Carlo method. This method is particularly onerous computationally, because it involves repeating the following steps a substantial number K of times: (i) draw one sample value from each of the 11 Poisson distributions whose means are the values $\hat{I}(1)$, $\hat{I}(8)$, $\dots$, $\hat{I}(71)$ corresponding to the solution of equations (7) for $\beta = \hat{\beta}$, $\gamma = \hat{\gamma}$ and $S_0 = \hat{S}_0$; (ii) estimate the same parameters, again via maximum likelihood, using the simulated draws, and compute the corresponding value of the basic reproduction number.

A sample of modest size $K = 1000$ drawn from the probability distribution of R_0 as just described (figure 2, right) had standard deviation 0.12, which is used as the standard uncertainty $u(R_0)$ associated with R_0 . A 95 % coverage interval for R_0 deduced from the sample ranged from 2.2 to 2.7.

8 Choosing the form of the measurement model

8.1 General

8.1.1 The same measurement principle can give rise to different models. Therefore, the experimenter is often faced with the need to choose a suitable form for the model from various possible forms. This clause gives guidance on the criteria that can be used in making this choice. Some of the forms of model are considered, with examples, in clause 13.

8.1.2 A measurement model should be capable of accounting for all information that is relevant and available. The following aspects should be taken into consideration when choosing the form of the model (for further information or specific guidance, see the referenced subclauses):

Availability of a reliable theoretical form The extent to which a model can be based on the measurement principle, usually a well-established scientific law, should be considered. A model based on a reliable scientific principle is likely to require less work to check its adequacy than does an empirical or hybrid model. See clauses 7 and 12.

Target measurement uncertainty The target measurement uncertainty affects the degree of approximation that is appropriate, and will also affect the number of corrections, etc. taken into consideration (see JCGM 200, 2.34).

Simplicity It may be important to provide a model that can be implemented with minimal effort. Simpler representations can also help to avoid mistakes in implementation. The use of sub-models (see 8.4) can be useful in this respect. See 9.2.

Measurement range The model should be applicable over the whole range of values of the input and output quantities over which it is intended to be used. See 5.8. It may be appropriate to divide the range into subranges in each of which a different model applies. See the example in 7.2.2. Also see clause 12.

Dominant sources of uncertainty Where the dominant uncertainties arise from measurement of input quantities, models that associate uncertainties with input quantities are most appropriate. Where the dominant uncertainties relate to unpredictable or random variation in observations, models incorporating performance data are usually more appropriate. See annex C.5.

Relevance A model that generates coefficient or parameter values that can be interpreted in terms of physical quantities can be easier for users to apply than a model that for mathematical simplicity uses abstract functions of physical quantities.

Parsimony If a statistical model is fitted to data, the model should not include more terms than necessary. This aspect is often addressed by the statistical process of model selection. See 11.10.

Available information The availability of comprehensive data on performance of the measurement procedure can make it possible to use simplified measurement models. See 10.3 and annex C.5.

Numerical accuracy The model should be numerically as 'well-posed' as possible, that is, not adversely affected by the limitations of the available computational precision. See 8.6.

Solution stability Some models requiring numerical solution (and particularly some representations) can lead to unstable numerical performance. Models that lead to stable solutions are preferred. See 8.6.

Computational cost Models that are easier to evaluate or solve with adequate accuracy (see 13.3 and 13.4) are often preferred to those that might require considerable computational effort (see 13.5 and 13.6).

8.1.3 The aspects listed in 8.1.2 are often mutually incompatible. For instance, the simplest model is rarely the most accurate, and the most tractable mathematical form may not be easy to interpret. Choice of model is therefore a balance depending on local priorities. The overriding concern is whether the model is capable of providing a valid estimate together with an associated measurement uncertainty. When a target measurement uncertainty is available, the model should be capable of providing results consistent with it.

8.1.4 Consideration should be given to choosing the most appropriate form of model, as different models may be appropriate for different purposes. Example 1 in this subclause is concerned with two models, the choice of which is made on the basis of providing data for different physical properties. Example 2 illustrates the advisability of using an implicit model when it provides a more natural description of the measurement. It also emphasizes that both algebraically and numerically an implicit model might have advantages over an explicit model. The example on shell thickness of microscopic spherical particles in 13.5 demonstrates a case in which it is not possible to transform an implicit model into an explicit model. Such a situation is common.

EXAMPLE 1 *Saturated vapour pressure* (also see 7.3.1)

The dependence of vapour pressure p at saturation on thermodynamic temperature T is often used as the basis for determining and predicting the volumetric properties of fluids. A differential equation, the Clausius-Clapeyron equation (6) defines the first derivative dp/dT of the saturated vapour pressure curve. A solution to this equation is the Antoine equation [7], a measurement model that takes the form

$$\ln \frac{p}{p_0} = A - \frac{B}{T + C}, \quad (8)$$

where p_0 is a reference pressure and A , B and C are coefficients, usually obtained by least-squares adjustment of vapour pressure data.

A different solution of the Clausius-Clapeyron equation, the Clarke and Glew equation [34], gives an alternative measurement model that relates vapour pressure data to thermodynamic functions:

$$R \ln \frac{p}{p_0} = -\frac{\Delta G^0(\Theta)}{\Theta} + \Delta H^0(\Theta) \left(\frac{1}{\Theta} - \frac{1}{T} \right) + \Delta C_p^0 \left(\frac{\Theta}{T} - 1 - \ln \frac{\Theta}{T} \right), \quad (9)$$

where R is the gas constant, Θ denotes a reference temperature, $\Delta G^0(\Theta)$ and $\Delta H^0(\Theta)$ are the molar free enthalpy and molar enthalpy differences between the vapour and the liquid phases at the temperature Θ , and ΔC_p^0 is the difference in molar heat capacity between the two phases.

Whereas measurement model (8), within a stated temperature range, conveniently reproduces experimental data within experimental uncertainty and interpolates vapour pressure data adequately, measurement model (9) is preferred when deriving thermodynamic properties from such data.

EXAMPLE 2 *Pressure generated by a pressure balance* (also see example 2 in 7.2.1)

Expression (3) in example 2 in 7.2.1 is a measurement model that defines implicitly the pressure p generated by a pressure balance. This model may equivalently be expressed as a quadratic equation

$$ap^2 + bp + c = 0 \quad (10)$$

in p , where

$$a = A_0 \lambda [1 + \alpha(T - T_{\text{ref}})], \quad b = A_0 [1 + \alpha(T - T_{\text{ref}})], \quad c = -m \left(1 - \frac{\rho_a}{\rho_m} \right) g,$$

with solution in the form of the explicit model

$$p = \frac{\sqrt{b^2 - 4ac} - b}{2a}. \quad (11)$$

Expression (11) is one of the two roots $(-b \pm \sqrt{b^2 - 4ac})/(2a)$ of equation (10), and is positive since a is positive and the term $4ac$ is negative. The other root is negative, carrying no physical meaning. Also see example 4 in 8.6.5.

In some situations it might be necessary to use the measurement model

$$p = \frac{m \left(1 - \frac{\rho_a}{\rho_m} \right) g}{A_0 (1 + \lambda p + \gamma p^2) [1 + \alpha(T - T_{\text{ref}})]},$$

that is, with a polynomial of degree two (or higher) replacing the term $1 + \lambda p$ in measurement model (3).

Consequently, the output quantity p corresponds to a root of a polynomial equation of degree at least 3, and it becomes more difficult (or impossible for degrees > 4) to derive an explicit measurement model for p in this case. Also see reference [40].

To an approximation that may be sufficient for the case in hand, p on the right-hand side of expression (3) can be replaced by a nominal value [113], and the measurement treated as explicit (see 13.3).

More complete measurement models can also be considered [113] that include, for instance, a correction to account for surface tension effects.

8.1.5 In calibration the relationship between the response variable and the stimulus variable can often be modelled using a polynomial of modest degree, often a straight line (polynomial of degree 1). Guidance on using a particular representation of polynomials (also see annex D), which assists in determining an appropriate polynomial degree, is available in ISO/TS 28038:2018 [99] and [37]. Also see example 2 in 8.3.3.

NOTE For many fields, specific guidance documents or international standards exist, providing advice on the selection of appropriate (polynomial) models for multipoint calibration.

8.1.6 In cases where there is more than one output quantity, the model should usually be treated as multivariate (see 13.4 and 13.6) rather than as separate univariate models (see 13.3 and 13.5) since knowledge is often required of covariances associated with the estimates of the output quantities. Instances arise in subsequent modelling and uncertainty evaluation and the determination of coverage regions (see JCGM 102:2011). Not taking such covariances into consideration generally leads to invalid statements of uncertainty.

EXAMPLE *Method of standard addition for determination of chemicals*

The method of standard addition is a popular way to estimate the concentration of various chemicals. It relies on partitioning a sample into several aliquots, adding to them known masses of a standard and measuring the analytical response from such spiked samples. A straight-line regression is determined from the data and the ratio of the intercept and the slope of this regression line estimates the amount of the analyte in the analyzed sample. Often the covariance between the intercept and the slope is neglected resulting in the uncertainty associated with the estimate from the method of standard addition being too small [121].

Data relating to the analysis of bromide in a water sample are

Mass fraction increment $x/\text{mg g}^{-1}$	0	47.8	95.6	142.8	190.7
Instrumental response y	1.775	2.676	3.578	4.418	5.316

The measurement model for the mass fraction of bromide in the analyzed water sample is $w = a/b$, where a and b are the coefficients of the straight-line regression $y = a + bx$. Application of ordinary least squares gives estimated coefficients $\hat{a} = 1.786$ and $\hat{b} = 0.018\,52\text{ g mg}^{-1}$ with associated standard uncertainties and covariance

$$u(\hat{a}) = 0.012\,4, \quad u(\hat{b}) = 0.000\,106\text{ g mg}^{-1}, \quad u(\hat{a}, \hat{b}) = -1.08 \times 10^{-6}\text{ g mg}^{-1}.$$

Alternatively, the correlation coefficient $r(\hat{a}, \hat{b}) = u(\hat{a}, \hat{b})/[u(\hat{a})u(\hat{b})] = -0.817$ can be reported. If the coefficients of the straight-line regression are treated as the output quantities obtained independently from two univariate models, the estimate of w is $\hat{w} = 96.4\text{ mg g}^{-1}$ with associated standard uncertainty $u(\hat{w}) = 0.9\text{ mg g}^{-1}$ given by the law of propagation of uncertainty. If, however, the correlation between a and b is (correctly) taken into consideration, the standard uncertainty is appreciably larger: $u(\hat{w}) = 1.2\text{ mg g}^{-1}$.

It is important to note that in this instance the data cannot be “mean-centred” (that is shifted with respect to x such that the arithmetic mean of the shifted x -values is zero), with a resulting zero correlation, before fitting the straight line. Doing so would yield a value $\hat{a}$ different from that required.

8.2 Fitness for purpose and approximations

8.2.1 Ideally, a basic measurement model should describe a scientific law or relation known to hold for the true values of the input quantities and the output quantities. In practice, the measurement model usually represents only a practicable, fit-for-purpose approximation of the ideal relationship. This is so because, although that relationship may be known, it may be too complicated or inconvenient for practical use. Alternatively, the relationship may be unknown, but an empirical approximation to it may be sufficient for the intended purpose. In some instances, it may be possible to use a close approximation to the ideal relationship on a small number of occasions, and also work with a somewhat inferior model that would be more practical for routine use.

8.2.2 It is generally inadvisable to select a model purely for convenience, for example, because it results in a simpler analysis or software is available for its implementation. In exceptional cases, it is accepted that analysis can be difficult, or software is unavailable or hard to develop. In such a circumstance, where a simpler model is used, there will be an uncertainty associated with the estimate of the measurand resulting from that use, which should be determined to the extent possible, and a corresponding term included in the measurement model. See [11.10](#) concerned with model uncertainty.

8.3 Representation and transformation of models

8.3.1 Parametrization

Parametrization is the process of representing or expressing a measurement model, whether theoretical or empirical, in terms of its quantities or parameters. For some models (especially theoretical models) it is important to retain the contextual meaning of the parameters. Some parametrizations can be more convenient operationally, some more in

accordance with working practices and some more reliable numerically (see 8.6). Transformations of the parameters in a measurement model, or re-parametrizations, are frequently applied in metrology to re-express a measurement result in an alternative form for purposes of communication or to yield a simpler (or numerically more stable) computation. In the latter case, the results of the computation are transformed back to the original formulation. Great care should be taken when establishing and propagating uncertainties following transformation (see 8.3.6).

EXAMPLE 1 *Straight line in terms of Cartesian (x, y) co-ordinates*

A straight line can be represented in Cartesian co-ordinates as

$$y = a + bx, \quad (12)$$

with parameters a and b , where a is the intercept on the y -axis and b is the slope. This parametrization is appropriate when describing functional relationships between quantities.

EXAMPLE 2 *Straight line in terms of polar (r, θ) co-ordinates*

The same line can also be represented as

$$x \sin \theta + y \cos \theta = \rho,$$

with parameters θ and ρ , where θ is the angle between the line and the horizontal and ρ is its distance of nearest approach to the origin. This parametrization can be useful when modelling geometrical problems where the line may be near-vertical, since b diverges while θ remains finite.

8.3.2 Re-parametrization

Re-parametrization of a measurement model is the use of a different set of parameters that depend in some manner on the original parameters. For unchanged values of the input quantities the values of the output quantities are unchanged following re-parametrization.

EXAMPLE *Straight line in terms of shifted coordinates*

An alternative to the line (12) makes use of *shifted* coordinates:

$$y - y_0 = a_0 + b(x - x_0), \quad (13)$$

with parameters a_0 and b , where x_0 and y_0 are selected in some convenient way. The expression of the line (13) as $y = (y_0 + a_0 - bx_0) + bx$ exposes the relationship between the original and new parametrization. The slope parameter b is unchanged. It can sometimes be useful to work in terms of *shifted and scaled* coordinates such as

$$x_{\text{new}} = \frac{x - x_0}{s}$$

for suitable choices of x_0 and s .

8.3.3 Use in regression

Suppose $x_i, y_i, i = 1, \dots, m$, represent measured coordinates of some underlying straight-line relationship. The use of representation (13) is often more desirable than the use of (12) since adverse numerical effects in the calculation can be more readily avoided.

EXAMPLE 1 *Drifting resistance standard* (also see 10.6.4)

The straight-line regression line in 10.6.4 is based on the shifted and scaled quantity

$$y = \frac{R - R_{\text{nom}}}{R_{\text{nom}}}$$

rather than the original quantity R . The values y_i of y (given in table 5 in 10.6.4) range from 17.9008 to 18.6916, whereas the corresponding values R_i of R range from 200.003580 to 200.003738. The former with dynamic range 1.04 (the ratio of the range endpoint values) are considerably more manageable than the latter (dynamic range 1.0000008).

EXAMPLE 2 *Thermoelectric voltage*

This example illustrates a circumstance in which the Chebyshev representation [37] of a polynomial function confers considerable advantages over the often-used monomial representation. The monomial and Chebyshev representations (annex D) of thermoelectric voltage are, respectively,

$$E = \sum_{r=0}^n c_r \vartheta^r, \quad E = \sum_{r=0}^n a_r T_r(t), \quad (14)$$

in the reference function for Type S thermocouples, for Celsius temperatures ϑ in the interval $[-50^\circ\text{C}, 1064.18^\circ\text{C}]$. The first of these expressions is given in [83] and the second is a re-parametrization of the first. The variable t in the right-hand expression (14) is given by

$$t = \frac{2\vartheta - \vartheta_{\min} - \vartheta_{\max}}{\vartheta_{\max} - \vartheta_{\min}} \quad (15)$$

and $T_r(t)$ denotes the Chebyshev polynomial of degree r in t (see annex D). There is a factor of some 10^{21} between the estimated non-zero coefficients $\hat{c}_r$ of largest and smallest magnitude in the monomial form, which are held to 12 significant decimal digits (12S): presumably it was considered that care is needed in working with this particular representation. The $\hat{c}_r$ are given to 5S in column 2 of table 1.

Table 1: Estimated polynomial coefficients for a Type S thermocouple

r	Raw, $\hat{c}_r/\text{mV}^\circ\text{C}^{-r}$	Scaled, $\hat{d}_r$	Normalized, $\hat{b}_r$	Chebyshev, $\hat{a}_r$
0	0	0	4.3036	4.6391
1	5.4031×10^{-3}	5.7499	5.5278	5.3711
2	1.2593×10^{-5}	14.2618	0.4784	0.3706
3	-2.3248×10^{-8}	-28.0174	-0.0543	-0.0729
4	3.2203×10^{-11}	41.3005	0.2206	0.0371
5	-3.3147×10^{-14}	-45.2390	-0.1637	-0.0130
6	2.5574×10^{-17}	37.1447	0.0216	0.0022
7	-1.2507×10^{-20}	-19.3310	-0.0249	-0.0004
8	2.7144×10^{-24}	4.4648	0.0252	0.0002

A scaled variable $q = \vartheta/B$ has been used in ITS-90 in recent years, where in this instance $B = 1064.18^\circ\text{C}$ is the upper endpoint of the interval of definition. Then, $E = \sum_{r=0}^n d_r q^r$, with $d_r = B^r c_r$. The scaling implies that the contribution from the r th term in the sum is bounded in magnitude by $|d_r|$. Values of E in mV are typically required to 3D (three decimal places). Accordingly, estimates $\hat{d}_r$ of the coefficients d_r are given in column 3 of table 1 to 4D (that is, including an extra digit) and are much more manageable. Alternatively, the variable can be normalized to the interval $[-1, 1]$ using the transformation (15) with $\vartheta_{\min} = -50^\circ\text{C}$ and $\vartheta_{\max} = B$. Estimates $\hat{b}_r$ of the corresponding coefficients b_r are given in column 4 and estimates $\hat{a}_r$ of the Chebyshev coefficients a_r in column 5 of table 1, both to 4D, obtained using references [35, 158].

Figure 3 depicts the reference function (14). It curves only gently, but the non-linearity present cannot be ignored. The estimated coefficients in the monomial representation in terms of the raw or scaled variable in table 1 give no indication of the gently curved form in figure 3. However, in strong contrast, for the normalized and Chebyshev forms, the dominance of the magnitudes of the first two estimated coefficients indicate that the calibration function has an appreciable linear (straight-line) component. The Chebyshev coefficients for degrees 7 and 8 could arguably be replaced by zero, since to 3D they make little contribution, with the degree of the polynomial consequently reduced from 8 to 6. Such reasoning could not be applied to the other polynomial representations.

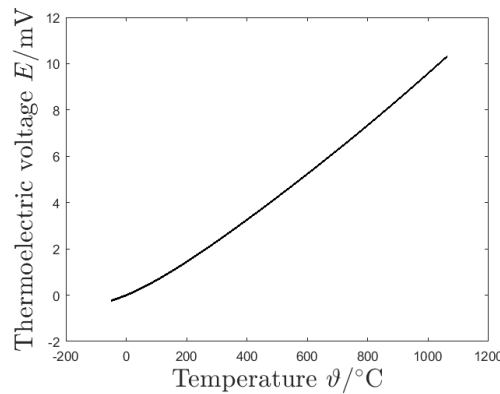


Figure 3: Relationship between temperature and thermoelectric voltage

8.3.4 Simple transformations

Some measurement models constitute simply transformation of the quantities involved ('transformation of variables').

EXAMPLE *Logarithmic and linear formats*

In radio-frequency and microwave electrical metrology, transformations are often made between logarithmic and linear representations of dimensionless reflection and transmission coefficients (scattering parameters or S-parameters). For an n -port electrical device, the expression is

$$\alpha = -20 \log_{10} |S|,$$

where $|S|$ is the modulus of a (complex-valued) linear S-parameter and α is the corresponding logarithmic loss (that is, return loss or attenuation), measured in dB.

$|S|$ is defined as

$$|S| = (x^2 + y^2)^{1/2},$$

where x and y are the real and imaginary components of the linear S-parameter.

In this example, measured values of x and y are $\hat{x} = 0.0060$ and $\hat{y} = 0.0080$ and their stated associated standard uncertainties are $u(\hat{x}) = u(\hat{y}) = 0.0100$. An estimate $|\hat{S}|$ of $|S|$ and thence $|\hat{\alpha}|$ of α are obtained:

$$|\hat{S}| = (\hat{x}^2 + \hat{y}^2)^{1/2} = 0.0100, \quad \hat{\alpha} = -20 \log_{10} |\hat{S}| = 40.0 \text{ dB}.$$

These values typify the measurement of the linear reflection coefficient of a near-matched (that is, low-reflecting) device.

Applying the law of propagation of uncertainty (LPU) (JCGM 100:2008, 5.1.2) gives

$$u(|\hat{S}|) = \frac{[\hat{x}^2 u^2(\hat{x}) + \hat{y}^2 u^2(\hat{y})]^{1/2}}{|\hat{S}|} = 0.0100, \quad \hat{u}(\alpha) = \frac{20}{\ln 10} \frac{u(|\hat{S}|)}{|\hat{S}|} = 8.7 \text{ dB}. \quad (16)$$

The appropriateness of formula (16) for the standard uncertainty $u(|\hat{S}|)$ is considered by also evaluating this uncertainty by applying the Monte Carlo method given in JCGM 101:2008. Application of this method with $M = 10^8$ trials, assuming x and y are independently normally distributed with means $\hat{x}$ and $\hat{y}$, standard deviations $u(\hat{x})$ and $u(\hat{y})$, and no correlation between x and y , gives the entries in column 3 of table 2, which are not in close agreement with the entries in column 2.

Table 2: Data and results for a logarithmic transformation using the law of propagation of uncertainty (LPU) and a Monte Carlo method (MC)

	$u(\hat{x}) = u(\hat{y}) = 0.01$		$u(\hat{x}) = u(\hat{y}) = 0.005$	
	LPU	MC	LPU	MC
$ \hat{S} $	0.0100	0.0155	0.0100	0.0114
$u(\hat{S})$	0.0100	0.0078	0.0050	0.0046
$\hat{\alpha}/\text{dB}$	40.0	37.6	40.0	39.8
$u(\hat{\alpha})/\text{dB}$	8.7	5.4	4.3	4.4

The M values of $|\hat{S}|$ given by these trials can be used to construct a histogram, which when scaled appropriately, as described in JCGM 101:2008, 7.5.2, would give an approximation (which would improve as M is increased) to the probability density function (PDF) for $|\hat{S}|$. This PDF is asymmetric, unlike the normal distribution assumed by the GUM. MC is expected to be more reliable in such circumstances.

Consider now that $u(\hat{x}) = u(\hat{y}) = 0.0050$ (rather than 0.0100). The results are given in columns 4 and 5 of table 2. The difference between the outcomes from LPU and JCGM 101:2008 is now much less since the degree of approximation in the first-order Taylor expansion of the measurement function, which underpins LPU, is better over a shorter interval. Moreover, the PDF is less skewed.

In general, it is not recommended to perform uncertainty calculations using logarithmic quantities in, for example, dB. Logarithmic quantities should be converted to the equivalent linear format before performing uncertainty calculations.

8.3.5 Non-linear relationships

When a plot of data representing a relationship between two variables suggests an underlying non-linear behaviour, it is often possible to transform the raw data to make it ‘more linear’. Doing so allows linear regression techniques to be used more effectively with such data. Re-parametrization in such an instance relates to the fact that the straight-line representation of the transformed data implies a different representation from that for the raw data. Such transformations generally change the statistical structure of the problem (see 8.3.6).

8.3.6 Impact on uncertainties

For uncertainty propagation, not all algebraically equivalent models behave necessarily in the same way because they are not equivalent statistically. An algebraic transformation should be accompanied by a corresponding statistical transformation to ensure the

integrity of the results obtained. The use of the law of propagation of uncertainty (JCGM 100:2008, 5.1.2) for this purpose is inadequate in some situations. Since the law of propagation of uncertainty is based on a linearization of the model, if errors originally followed a certain distribution, in the transformed problem they would generally follow a different distribution. Transformations have an impact on the uncertainties associated with the estimates of the quantities involved or on the weights in a statistical regression analysis involving such a model. See the example in 8.3.4.

NOTE Transformations also have an impact on the probability distributions used to characterize the quantities involved [129].

EXAMPLE *Re-parametrization of a model for lead adsorption by nano-particles*

The Langmuir adsorption model [111] describes the theoretical relation between the amount concentration Γ of a solute on the surface of an adsorbent to the amount concentration c of the solute in the liquid with which it is in contact:

$$\Gamma = \Gamma_{\max} \frac{Kc}{1 + Kc}, \quad (17)$$

where K is the Langmuir binding-strength coefficient and $\Gamma_{\max}$ (the measurand) is the maximum sorption capacity of the adsorbent. A reparametrized form of the Langmuir model is often used based on taking the reciprocal of both sides of model (17), which expresses $1/\Gamma$ as a linear function of $1/c$:

$$\frac{1}{\Gamma} = \frac{1}{\Gamma_{\max}} + \frac{1}{\Gamma_{\max}K} \times \frac{1}{c}. \quad (18)$$

The model parameters $1/\Gamma_{\max}$ and $1/(\Gamma_{\max}K)$ can be obtained by linear regression. Although models (17) and (18) are mathematically equivalent, different results are obtained for $\Gamma_{\max}$.

Consider measured values of c equal to

$$0.20 \text{ mmol L}^{-1}, \quad 0.25 \text{ mmol L}^{-1}, \quad 0.33 \text{ mmol L}^{-1}, \quad 0.60 \text{ mmol L}^{-1}, \quad 2.00 \text{ mmol L}^{-1},$$

and corresponding measured values of Γ equal to

$$9.4 \text{ mmol g}^{-1}, \quad 11.1 \text{ mmol g}^{-1}, \quad 13.9 \text{ mmol g}^{-1}, \quad 20.0 \text{ mmol g}^{-1}, \quad 33.3 \text{ mmol g}^{-1}.$$

Assuming c and Γ are independent, and not accounting for measurement uncertainties associated with Γ and c in order to illustrate the point, $\hat{\Gamma}_{\max} = 46.4 \text{ mmol g}^{-1}$ with associated standard uncertainty $u(\hat{\Gamma}_{\max}) = 0.3 \text{ mmol g}^{-1}$ is obtained by non-linear least-squares regression using expression (17).

Ordinary least-squares (OLS) fitting using expression (18) gives $1/\hat{\Gamma}_{\max} = 0.0214 \text{ g mmol}^{-1}$ with associated standard uncertainty $u(1/\hat{\Gamma}_{\max}) = 0.0006 \text{ g mmol}^{-1}$, which following reciprocation corresponds to $\hat{\Gamma}_{\max} = 46.7 \text{ mmol g}^{-1}$ with associated standard uncertainty $u(\hat{\Gamma}_{\max}) = 1.4 \text{ mmol g}^{-1}$.

Several other linearized versions of model (17) exist; it is emphasized that re-parametrization can have a significant effect on the results if the transformed uncertainties are obtained using the law of propagation of uncertainty, which assumes sufficiently accurate linearizability. Although both models are *algebraically* equivalent, OLS treatment of these models differs in its assumptions. The OLS treatment of (17) implies normality in the dispersion of Γ values whereas OLS treatment of (18) implies normality in the dispersion of $1/\Gamma$ values. These assumptions are inconsistent.

Although the values of $\hat{\Gamma}_{\max}$ obtained by the two methods are consistent with respect to their associated standard uncertainties, this may not be the case in other circumstances.

8.3.7 Explicit and implicit forms of measurement model

When it is possible to transform an implicit expression to an explicit expression, there can be a preferred choice that depends on the particular circumstances. Sometimes an implicit form is preferable because it can have better numerical behaviour even when an explicit form can be deduced from it.

EXAMPLE *Representation of a circle*

In the assessment of geometric form in dimensional metrology [6] the equation for the co-ordinates (x, y) of a point on a circle centred at (a, b) with radius r is written implicitly as expression $(x - a)^2 + (y - b)^2 = r^2$. Then, y expressed explicitly in terms of the other quantities is given by expression $y = b \pm [r^2 - (x - a)^2]^{1/2}$. Because of subtractive cancellation the use of the latter expression becomes problematic when $|x - a| \approx r$. Alternatively, a convenient way to represent a circle is through the use of a parameter θ :

$$x = a + r \cos \theta, \quad y = b + r \sin \theta,$$

which is appropriate and numerically stable for values of θ between 0 and 2π and all co-ordinates (x, y) .

8.4 Multi-stage measurement models

8.4.1 In many stepwise processes in metrology, quantities from intermediate measurements are naturally used in a subsequent measurement. Each stage in the process can be described by a measurement model with input quantities and output quantities. This set of measurement models constitutes a multi-stage measurement model and can be used as such. Equivalently, the complete process can sometimes conveniently be described by a single-stage measurement model, perhaps involving a different number of quantities.

8.4.2 Multi-stage models also arise as a natural consequence of the dissemination chain connecting ideally all kinds of measurements to the relevant SI units. Sometimes, to evaluate correctly the uncertainty associated with an estimate of the output quantities at a given stage, it is necessary to consider the previous stages in connection with the current stage. By implication, it can be necessary to consider the corresponding measurement models as a single multi-stage measurement model. An instance arises in mass and force measurements, in which covariances between volume and mass at the various stages of the dissemination chain must be taken into account to evaluate correctly the contribution of the buoyancy correction to the uncertainty associated with the output estimate of the current calibration [118].

EXAMPLE 1 *How long is a piece of string?*

Consider the problem of establishing a model for the measurement of the length L of a piece of string using a steel tape. Inevitably, idealizations and approximations are necessary. A simpler treatment involving fewer factors is available [15]. The measurand is the length L . It depends on several input quantities representing the observed string length and corrections to that length. Most of these quantities are expressed in terms of other quantities. The measurement model takes the form

String length = Observed string length (A)
 + Steel tape length correction (B)
 + String length correction (C)
 + Measurement process correction (D),

where

(A)	Observed string length	=	Average of a number of repeated observations (Q_{11})
(B)	Steel tape length correction	=	[Length deviation due to tape calibration imperfections (Q_{21}) + Extension in tape due to stretching (this correction is negative if there is shrinking rather than stretching) (Q_{22}) + Reduction in effective length of tape due to bending of the tape (Q_{23})] × Multiplicative correction for steel tape thermal expansion (Q_{24})
(C)	String length correction	=	Reduction in effective string length due to string departing from a straight line (Q_{31}) + Reduction in string length as a result of shrinking (negative if there is stretching rather than shrinking) (Q_{32})
(D)	Measurement process correction	=	Length deviation due to inability to align end of tape with end of string due to fraying of the string ends (Q_{41}) + Length deviation due to tape and string not being parallel (Q_{42}) + Length deviation due to reading a numerical value from the tape (Q_{43}).

The measurement model is thus expressed symbolically as

$$L = Q_{11} + (Q_{21} + Q_{22} + Q_{23})Q_{24} + (Q_{31} + Q_{32}) + (Q_{41} + Q_{42} + Q_{43}).$$

Each input quantity Q_{ij} would have an estimate and associated standard uncertainty, or be characterized by an appropriate probability distribution depending on the knowledge available. In the latter case, for instance, (a) a scaled and shifted t distribution is used for the quantity Q_{11} corresponding to the observed string length, based on repeated observations (see JCGM 101:2008, 6.4.9), and (b) a distribution based on a circular-arc model is used for the quantity Q_{23} . This example is continued in example 1 in 10.4.3.

The distribution for Q_{23} is related to the chi-squared distribution and does not have zero expectation, since the *minimum* effect of tape bending on the output quantity is zero. This degree of sophistication would not be warranted when measuring the length of a piece of string, but relevant in some other applications.

This example can be interpreted as a multi-stage model with the quantities representing the steel-tape-length correction, string-length correction and measurement-process correction described by sub-models.

EXAMPLE 2 *Peak area determined from spectral data*

A requirement in spectroscopy is the detection of peaks in a signal and the determination of peak parameters such as area and location. The effects of noise in the signal are reduced by first smoothing the data. Peak area can be considered in terms of a two-stage model or a single-stage model.

Two-stage model In a first stage data, with associated standard uncertainties, are filtered using a windowing function, of rectangular or triangular form, for instance. The result of the filtering is a set of smoothed values, with associated standard uncertainties and covariances. At least