BRITISH STANDARD

BS ISO 11929:2010

Determination of the characteristic limits (decision threshold, detection limit and limits of the confidence interval) for measurements of ionizing radiation — Fundamentals and application

ICS 17.240

BSI British Standards

National foreword

This British Standard is the UK implementation of ISO 11929:2010. It supersedes BS ISO 11929-1:2000, BS ISO 11929-2:2000, BS ISO 11929-3:2000, BS ISO 11929-4:2001, BS ISO 11929-5:2005, BS ISO 11929-6:2005, BS ISO 11929-7:2005 and BS ISO 11929-8:2005, which are withdrawn.

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INTERNATIONAL STANDARD

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Determination of the characteristic limits (decision threshold, detection limit and limits of the confidence interval) for measurements of ionizing radiation — Fundamentals and application

Détermination des limites caractéristiques (seuil de décision, limite de détection et extrémités de l'intervalle de confiance) pour mesurages de rayonnements ionisants — Principes fondamentaux et applications

Reference number
ISO 11929:2010(E)

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Foreword

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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 11929 was prepared by Technical Committee ISO/TC 85, *Nuclear energy*, Subcommittee SC 2, *Radiation protection*.

This first edition of ISO 11929 cancels and replaces ISO 11929-1:2000, ISO 11929-2:2000, ISO 11929-3:2000, ISO 11929-4:2001, ISO 11929-5:2005, ISO 11929-6:2005, ISO 11929-7:2005 and ISO 11929-8:2005, which have been technically revised, specifically with reference to the type of statistical treatment of the data.

Introduction

The limits to be provided according to this International Standard by means of statistical tests and specified probabilities allow detection possibilities to be assessed for a measurand and for the physical effect quantified by this measurand as follows:

— the “decision threshold” gives a decision on whether or not the physical effect quantified by the measurand is present;

— the “detection limit” indicates the smallest true value of the measurand which can still be detected with the applied measurement procedure; this gives a decision on whether or not the measurement procedure satisfies the requirements and is therefore suitable for the intended measurement purpose;

— the “limits of the confidence interval” enclose, in the case of the physical effect recognized as present, a confidence interval containing the true value of the measurand with a specified probability.

Hereinafter, the limits mentioned are jointly called “characteristic limits”.

Since measurement uncertainty plays an important part in this International Standard, the evaluation of measurements and the treatment of measurement uncertainties are carried out by means of the general procedures according to ISO/IEC Guide 98-3; see also References [1, 2]. This enables the strict separation of the evaluation of the measurements, on the one hand (Clause 5), and the provision and calculation of the characteristic limits, on the other hand (Clause 6). This International Standard is based on Bayesian statistics according to References [6 to 19], such that uncertain quantities and influences, which do not behave randomly in measurements repeated several times or in counting measurements, can also be taken into account.

Equations are provided for the calculation of the characteristic limits of an ionizing radiation measurand via the “standard measurement uncertainty” of the measurand (hereinafter “standard uncertainty”). The standard uncertainties of the measurement, as well as those of sample treatment, calibration of the measuring system and other influences are taken into account. However, the latter standard uncertainties are assumed to be known from previous investigations.

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INTERNATIONAL STANDARD **ISO 11929:2010(E)**

Determination of the characteristic limits (decision threshold, detection limit and limits of the confidence interval) for measurements of ionizing radiation — Fundamentals and application

1 Scope

This International Standard specifies a procedure, in the field of ionizing radiation metrology, for the calculation of the "decision threshold", the "detection limit" and the "limits of the confidence interval" for a non-negative ionizing radiation measurand, when counting measurements with preselection of time or counts are carried out, and the measurand results from a gross count rate and a background count rate as well as from further quantities on the basis of a model of the evaluation. In particular, the measurand can be the net count rate as the difference of the gross count rate and the background count rate, or the net activity of a sample. It can also be influenced by calibration of the measuring system, by sample treatment and by other factors.

This International Standard also applies, in the same way to:

— counting measurements on moving objects (see B.2);

— measurements with linear-scale analogue count rate measuring instruments (hereinafter called ratemeters, see B.3);

— repeated counting measurements with random influences (see B.4);

— counting measurements on filters during accumulation of radioactive material (see B.5);

— counting spectrometric multi-channel measurements, if particular lines in the spectrum are to be considered and no adjustment calculations, for instance, an unfolding, have to be carried out (see C.2 to C.4);

— counting spectrometric multi-channel measurements if evaluated by unfolding methods (see C.5), in particular, alpha- and gamma-spectrometric measurements (see C.5.5 and C.5.6, respectively).

This International Standard also applies analogously to other measurements of any kind if the same model of the evaluation is involved. In this sense, it is also applicable to measurements with albedo dosimeters [18]. Further practical examples can be found in other International Standards, for example ISO 18589[21], ISO 9696[22], ISO 9697[23], ISO 9698[24], ISO 9699[25], ISO 10703[26], ISO 7503[27] and ISO 28218[28].

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 31-0, *Quantities and units — Part 0: General principles*

ISO 31-9, *Quantities and units — Part 9: Atomic and nuclear physics*

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ISO/IEC Guide 98-3:2008, *Uncertainty of measurement — Part 3: Guide to the expression of uncertainty in measurement (GUM:1995)*

ISO/IEC Guide 99:2007, *International vocabulary of metrology — Basic and general concepts and associated terms (VIM)*

ISO 3534-1, *Statistics — Vocabulary and symbols — Part 1: General statistical terms and terms used in probability*

3 Terms and definitions

For the purposes of this document, the terms and definitions given in ISO 31-0, ISO 31-9, ISO/IEC Guide 98-3, ISO/IEC Guide 99 and ISO 3534-1 and the following apply.

3.1
measurement procedure
set of operations, described specifically, used in the performance of particular measurements according to a given method

[ISO/IEC Guide 99:2007, 2.6]

3.2
measurand
particular quantity subject to measurement

[ISO/IEC Guide 99:2007, 2.3]

NOTE In this International Standard, a measurand is non-negative and quantifies a nuclear radiation effect. The effect is not present if the true value of the measurand is zero. An example of a measurand is the intensity of an energy line in a spectrum above the background in a spectrometric measurement.

3.3
result of a measurement
value attributed to a measurand, obtained by measurement

[ISO/IEC Guide 99:2007, 2.9]

3.4
uncertainty of measurement
uncertainty
non-negative parameter, which characterizes the dispersion of the values which could reasonably be attributed to the measurand

[ISO/IEC Guide 99:2007, 2.26]

See also ISO/IEC Guide 98-3.

NOTE The uncertainty of a measurement derived according to ISO/IEC Guide 98-3 comprises, in general, many components. Some of these components can be evaluated from the statistical distribution of the results of series of measurements and can be characterized by experimental standard deviations. The other components, which can also be characterized by standard deviations, are evaluated from assumed or known probability distributions based on experience and other information.

3.5
model of evaluation
set of mathematical relationships between all measured and other quantities involved in the evaluation of measurements

NOTE The model of evaluation does not need to be an explicit function; it can also be an algorithm realized by a computer code.

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3.6
decision threshold
value of the estimator of the measurand, which when exceeded by the result of an actual measurement using a given measurement procedure of a measurand quantifying a physical effect, one decides that the physical effect is present

NOTE 1 The decision threshold is defined such that in cases where the measurement result, y, exceeds the decision threshold, y^*, the probability that the true value of the measurand is zero is less or equal to a chosen probability, α.

NOTE 2 If the result, y, is below the decision threshold, y^*, the result cannot be attributed to the physical effect; nevertheless it cannot be concluded that it is absent.

3.7
detection limit
smallest true value of the measurand which ensures a specified probability of being detectable by the measurement procedure

NOTE With the decision threshold according to 3.6, the detection limit is the smallest true value of the measurand for which the probability of wrongly deciding that the true value of the measurand is zero is equal to a specified value, β, when, in fact, the true value of the measurand is not zero.

3.8
limits of the confidence interval
values which define a confidence interval containing the true value of the measurand with a specified probability

NOTE A confidence interval is sometimes known as a credible interval or a Bayesian interval. It is characterized in this International Standard by a specified probability $(1-\gamma)$.

3.9
best estimate of the true value of the measurand
expectation value of the probability distribution of the true value of the measurand, given the experimental result and all prior information on the measurand

NOTE The best estimate, among all possible estimates of the measurand on the basis of given information, which is associated with the minimum uncertainty.

3.10
guideline value
value which corresponds to scientific, legal or other requirements and which is intended to be assessed by the measurement procedure

NOTE 1 The guideline value can be given, for example, as an activity, a specific activity or an activity concentration, a surface activity or a dose rate.

NOTE 2 The comparison of the detection limit with a guideline value allows a decision on whether or not the measurement procedure satisfies the requirements set forth by the guideline value and is therefore suitable for the intended measurement purpose. The measurement procedure satisfies the requirement if the detection limit is smaller than the guideline value.

3.11
background effect
measurement effect caused by radiation other than that caused by the object of the measurement itself

EXAMPLE Natural radiation sources.

3.12
net effect
contribution of the possible radiation of a measurement object (for instance, of a radiation source or radiation field) to the measurement effect

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3.13
gross effect
measurement effect caused by the background effect and the net effect

3.14
shielding factor
factor describing the reduction of the background count rate by the effect of shielding caused by the measurement object

3.15
relaxation time constant
duration in which the output signal of a linear-scale ratemeter decreases to 1/e times the starting value after stopping the sequence of the input pulses

3.16
background
⟨spectrometric measurements⟩ number of events of no interest in the region of a specific line in the spectrum

NOTE The events can be due to the background effect by the environmental radiation and also to the sample itself (for instance, from other lines).

4 Quantities and symbols

The symbols for auxiliary quantities and the symbols only used in the annexes are not listed. Physical quantities are denoted by upper-case letters but shall be carefully distinguished from their values, denoted by the corresponding lower-case letters. In addition, the special quantities and symbols for unfolding in spectrometric measurements given in C.5.1 and for Bayesian statistics given in F.2.1 are used.

m number of input quantities

X_i input quantity $(i = 1, ..., m)$

x_i estimate of the input quantity X_i

$u(x_i)$ standard uncertainty of the input quantity X_i associated with the estimate x_i

$h_1(x_1)$ standard uncertainty $u(x_1)$ as a function of the estimate x_1

Δx_i width of the region of the possible values of the input quantity X_i

$u_{\text{rel}}(w)$ relative standard uncertainty of a quantity Y_k associated with the estimate w

G model function

Y random variable as an estimator of the measurand; also used as the symbol for the non-negative measurand itself, which quantifies the physical effect of interest

$\tilde{y}$ true value of the measurand; if the physical effect of interest is not present, then $\tilde{y} = 0$; otherwise, $\tilde{y} > 0$

y determined value of the estimator Y, estimate of the measurand, primary measurement result of the measurand

y_j values y from different measurements $(j = 0, 1, 2, ...)$

$u(y)$ standard uncertainty of the measurand associated with the primary measurement result y

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$\tilde{u}(\tilde{y})$	standard uncertainty of the estimator Y as a function of the true value $\tilde{y}$ of the measurand
$\hat{y}$	best estimate of the measurand
$u(\hat{y})$	standard uncertainty of the measurand associated with the best estimate $\hat{y}$
y^*	decision threshold of the measurand
$y^\#$	detection limit of the measurand
$\tilde{y}_i$	approximations of the detection limit $y^\#$
y_r	guideline value of the measurand
$y^\triangleleft$, $y^\triangleright$	lower and upper limit of the confidence interval, respectively, of the measurand
ρ_i	count rate as an input quantity X_i
ρ_n	count rate of the net effect (net count rate)
ρ_g	count rate of the gross effect (gross count rate)
ρ_0	count rate of the background effect (background count rate)
n_i	number of counted pulses obtained from the measurement of the count rate ρ_i
n_g, n_0	number of counted pulses of the gross effect and of the background effect, respectively
t_i	measurement duration of the measurement of the count rate ρ_i
t_g, t_0	measurement duration of the measurement of the gross effect and of the background effect, respectively
r_i	estimate of the count rate ρ_i
r_g, r_0	estimate of the gross count rate and of the background count rate, respectively
τ_g, τ_0	relaxation time constant of a ratemeter used for the measurement of the gross effect and of the background effect, respectively
α, β	probability of the error of the first and second kind, respectively
$1-\gamma$	probability for the confidence interval of the measurand
k_p, k_q	quantiles of the standardized normal distribution for the probabilities p and q, respectively (for instance $p=1-\alpha$, $1-\beta$ or $1-\gamma/2$)
$\Phi(t)$	distribution function of the standardized normal distribution; $\Phi(k_p)=p$ applies

5 Fundamentals

5.1 General aspects concerning the measurand

A non-negative measurand shall be assigned to the physical effect to be investigated according to a given measurement task. The measurand shall quantify the effect. It assumes the true value $\tilde{y}=0$ if the effect is not present in a particular case.

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Then, a random variable Y, an estimator, shall be assigned to the measurand. The symbol Y is also used in this clause for the measurand itself. A value y of the estimator Y, determined from measurements, is an estimate of the measurand. It shall be calculated as the primary measurement result together with the primary standard uncertainty $u(y)$, of the measurand associated with y. These two values form the primary complete measurement result for the measurand and are obtained in accordance with ISO/IEC Guide 98-3 (see also References [1, 2]) by evaluation of the measurement data and other information by means of a model (of the evaluation), which mathematically connects all the quantities involved (see 5.2). In general, the fact that the measurand is non-negative is not explicitly taken into account in the evaluation. Therefore, y may be negative, especially when the measurand nearly assumes the true value $\tilde{y} = 0$. The primary measurement result, y, differs from the best estimate, $\hat{y}$, of the measurand calculated in 6.5. With $\hat{y}$, the knowledge that the measurand is non-negative is taken into account. The standard uncertainty, $u(\hat{y})$, associated with $\hat{y}$ is smaller than $u(y)$.

5.2 Model

5.2.1 General model

In many cases, the measurand, Y, is a function of several input quantities, X_i, in the form of Equation (1):

$$Y = G(X_1, ..., X_m) \tag{1}$$

Equation (1) is the model of the evaluation. Substituting given estimates, x_i, of the input quantities, X_i, in the model function, G, Equation (1) yields the primary measurement result y of the measurand as:

$$y = G(x_1, ..., x_m) \tag{2}$$

The standard uncertainty, $u(y)$, of the measurand associated with the primary measurement result, y, is calculated according to Equation (3), if the input quantities, X_i, are independently measured and standard uncertainties, $u(x_i)$, associated with the estimates, x_i, are given, from the relation:

$$u^2(y) = \sum_{i=1}^{m} \left(\frac{\partial G}{\partial X_i} \right)^2 u^2(x_i) \tag{3}$$

In Equation (3), the estimates, x_i, shall be substituted for the input quantities, X_i, in the partial derivatives of G. The determination of the estimates, x_i, and the associated standard uncertainties, $u(x_i)$, and also the numerical or experimental determination of the partial derivatives are in accordance with ISO/IEC Guide 98-3 or References [1, 2]. For a count rate, $X_i = \rho_i$, with the given counting result, n_i, recorded during the measurement of duration, t_i, the specifications $x_i = r_i = n_i / t_i$ and $u^2(x_i) = n_i / t_i^2 = r_i / t_i$ apply (see also F.1). If the input quantities are not independently measured and for more complicated measurement evaluations such as unfolding, see C.5.2.

In 5.2.2, the input quantity, X_1, for instance the gross count rate, is taken as that quantity whose value, x_1, is not given when a true value, $\tilde{y}$, of the measurand, Y, is specified within the framework of the calculation of the decision threshold and the detection limit. Analogously, the input quantity, X_2, is assigned in a suitable way to the background effect. The data of the other input quantities are taken as given from independent previous investigations.

5.2.2 Model in ionizing radiation measurements

In this International Standard, the measurand, Y, with its true value, $\tilde{y}$, relates to a sample of radioactive material and is determined from counting the gross effect and the background effect with preselection of time or counts. In particular, Y can be the net count rate, ρ_n, or the net activity, A, of the sample. The symbols belonging to the counting of the gross effect and of the background effect are marked in the following by the subscripts g and 0, respectively.

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In this International Standard, the model is specified as follows:

$$Y = G(X_1, ..., X_m) = (X_1 - X_2 X_3 - X_4) \cdot \frac{X_6 X_8 \cdots}{X_5 X_7 \cdots} = (X_1 - X_2 X_3 - X_4) \cdot W \tag{4}$$

with

$$W = \frac{X_6 X_8 \cdots}{X_5 X_7 \cdots} \tag{5}$$

$X_1 = \rho_g$ is the gross count rate and $X_2 = \rho_0$ is the background count rate. The other input quantities, X_i, are calibration, correction or influence quantities, or conversion factors, for instance the emission or response probability or, in particular, X_3 is a shielding factor and X_4 an additional background correction quantity. If some of the input quantities are not involved, $x_i = 1$ $(i = 3;\ i > 4)$, $x_4 = 0$ and $u(x_i) = 0$ shall be set for them. For the count rates, $x_1 = r_g = n_g / t_g$ and $u^2(x_1) = n_g / t_g^2 = r_g / t_g$ as well as $x_2 = r_0 = n_0 / t_0$ and $u^2(x_2) = n_0 / t_0^2 = r_0 / t_0$ apply.

By substituting the estimates, x_i, in Equation (4), the primary estimate, y, of the measurand, Y, gives the result:

$$y = G(x_1, ..., x_m) = (x_1 - x_2 x_3 - x_4) \cdot w = (r_g - r_0 x_3 - x_4) \cdot w = \left(\frac{n_g}{t_g} - \frac{n_0}{t_0} x_3 - x_4 \right) \cdot w \tag{6}$$

with

$$w = \frac{x_6 x_8 \cdots}{x_5 x_7 \cdots} \tag{7}$$

With the partial derivatives:

$$\frac{\partial G}{\partial X_1} = W\ ;\ \frac{\partial G}{\partial X_2} = -X_3 W\ ;\ \frac{\partial G}{\partial X_3} = -X_2 W\ ;\ \frac{\partial G}{\partial X_4} = -W\ ;\ \frac{\partial G}{\partial X_i} = \pm \frac{Y}{X_i} \quad (i \geqslant 5) \tag{8}$$

and by substituting the estimates x_i, w and y, Equation (3) yields the standard uncertainty $u(y)$ of the measurand associated with y:

$$\begin{aligned} u(y) &= \sqrt{w^2 \cdot \left[u^2(x_1) + x_3^2 u^2(x_2) + x_2^2 u^2(x_3) + u^2(x_4) \right] + y^2 u_{rel}^2(w)} \\ &= \sqrt{w^2 \cdot \left[r_g / t_g + x_3^2 r_0 / t_0 + r_0^2 u^2(x_3) + u^2(x_4) \right] + y^2 u_{rel}^2(w)} \end{aligned} \tag{9}$$

where

$$u_{rel}^2(w) = \sum_{i=5}^{m} \frac{u^2(x_i)}{x_i^2} \tag{10}$$

is the sum of the squared relative standard uncertainties of the quantities X_5 to X_m. For $m < 5$, the values $w = 1$ and $u_{rel}^2(w) = 0$ apply.

The estimate x_i and the standard uncertainty $u(x_i)$ of X_i $(i = 3, ..., m)$ are taken as known from previous investigations or as values of experience according to other information. In the previous investigations, x_i can be determined as an arithmetic mean value and $u^2(x_i)$ as an empirical variance (see B.4.1). If necessary,

$u^2(x_i)$ can also be calculated as the variance of a rectangular distribution over the region of the possible values of X_i with the width Δx_i. This yields $u^2(x_i) = (\Delta x_i)^2/12$.

For the application of the procedure to particular measurements, including spectrometric measurements, see Annexes B and C.

5.3 Calculation of the standard uncertainty as a function of the measurand

5.3.1 General aspects

For the provision and numerical calculation of the decision threshold in 6.2 and of the detection limit in 6.3, the standard uncertainty of the measurand is needed as a function $\tilde{u}(\tilde{y})$ of the true value $\tilde{y} \geqslant 0$ of the measurand. This function shall be determined in a way similar to $u(y)$ within the framework of the evaluation of the measurements by application of ISO/IEC Guide 98-3; see also References [1, 2]. In most cases, $\tilde{u}(\tilde{y})$ shall be formed as a positive square root of a variance function $\tilde{u}^2(\tilde{y})$ calculated first. This function shall be defined, unique and continuous for all $\tilde{y} \geqslant 0$ and shall not assume negative values.

In most cases, $\tilde{u}(\tilde{y})$ can be explicitly specified, provided that $u(x_1)$ is given as a function $h_1(x_1)$ of x_1. In such cases, y shall be formally replaced by $\tilde{y}$ and Equation (2) shall be solved for x_1. With a specified $\tilde{y}$, the value x_1 can also be calculated numerically from Equation (2); for instance, by means of an iteration procedure, which results in x_1 as a function of $\tilde{y}$ and x_2, ..., x_m. This function shall replace x_1 in Equation (3) and in $u(x_1) = h_1(x_1)$, which finally yields $\tilde{u}(\tilde{y})$ instead of $u(y)$. In the case of the model according to Equation (6) and 5.3.2, one shall proceed in this way. Otherwise, 5.3.3 shall be applied, where $\tilde{u}(\tilde{y})$ follows as an approximation by interpolation from the data y_j and $u(y_j)$ of several measurements.

5.3.2 Explicit calculation

When, in the case of the model according to Equation (6), the standard uncertainty, $u(x_1)$, of the gross count rate $X_1 = \rho_g$, is given as a function $h_1(x_1)$ of the estimate, $x_1 = r_g$, either $h_1(x_1) = \sqrt{x_1/t_g}$ or $h_1(x_1) = x_1/\sqrt{n_g}$ applies if the measurement duration, t_g (time preselection), or, respectively, the number, n_g, of recorded pulses (preselection of counts) is specified.

The value y shall be formally replaced by $\tilde{y}$. This allows the elimination of x_1 in the general case and, in particular, of n_g with time preselection and of t_g with preselection of counts in Equation (9) by means of Equation (6). These values are not available when $\tilde{y}$ is specified. This yields in the general case according to Equation (6)

$$x_1 = \tilde{y}/w + x_2 x_3 + x_4 \tag{11}$$

By substituting x_1 according to Equation (11) in the given function $h_1(x_1)$, i.e. with $u^2(x_1) = h_1^2(\tilde{y}/w + x_2 x_3 + x_4)$, the following results from Equation (9):

$$\tilde{u}(\tilde{y}) = \sqrt{w^2 \cdot \left[h_1^2(\tilde{y}/w + x_2 x_3 + x_4) + x_3^2 u^2(x_2) + x_2^2 u^2(x_3) + u^2(x_4) \right] + \tilde{y}^2 u_{\text{rel}}^2(w)} \tag{12}$$

With time preselection and because of $x_1 = n_g/t_g$ and $x_2 = r_0$,

$$n_g = t_g \cdot (\tilde{y}/w + r_0 x_3 + x_4) \tag{13}$$

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is obtained from Equation (11). Then, with $h_1^2(x_1) = x_1/t_g = n_g/t_g^2$ and by substituting n_g according to Equation (13) and with $u^2(x_2) = r_0/t_0$, Equation (12) leads to

$$\tilde{u}(\tilde{y}) = \sqrt{w^2 \cdot \left[(\tilde{y}/w + r_0 x_3 + x_4)/t_g + x_3^2 r_0/t_0 + r_0^2 u^2(x_3) + u^2(x_4) \right] + \tilde{y}^2 u_{rel}^2(w)} \tag{14}$$

With preselection of counts,

$$t_g = \frac{n_g}{\tilde{y}/w + r_0 x_3 + x_4} \tag{15}$$

is analogously obtained. Then, with $h_1^2(x_1) = x_1/t_g = n_g/t_g^2$ and by substituting t_g according to Equation (15) and with $u^2(x_2) = r_0^2/n_0$, Equation (12) leads to

$$\tilde{u}(\tilde{y}) = \sqrt{w^2 \cdot \left[(\tilde{y}/w + r_0 x_3 + x_4)^2/n_g + x_3^2 r_0^2/n_0 + r_0^2 u^2(x_3) + u^2(x_4) \right] + \tilde{y}^2 u_{rel}^2(w)} \tag{16}$$

Equation (22) has a solution, which is the detection limit, $y^{\#}$, if, with time preselection, the following condition is satisfied:

$$k_{1-\beta} u_{rel}(w) < 1 \tag{17}$$

or with preselection of counts, the following condition is satisfied:

$$k_{1-\beta} \cdot \sqrt{\frac{1}{n_g} + u_{rel}^2(w)} < 1 \tag{18}$$

Otherwise, it can happen that a detection limit does not exist because of too great an uncertainty of the quantities X_5 to X_m, summarily expressed by $u_{rel}(w)$. The condition according to Equation (17) also applies in the case of Equation (12) if $h_1(x_1)$ increases for growing x_1 more slowly than x_1, i.e. if $h_1(x_1)/x_1 \to 0$ for $x_1 \to \infty$.

5.3.3 Approximations

It is often sufficient to use the following approximations for the function $\tilde{u}(\tilde{y})$, in particular, if the standard uncertainty, $u(x_1)$, is not known as a function $h_1(x_1)$. A prerequisite is that measurement result, y_j , and associated standard uncertainties, $u(y_j)$, calculated according to 5.1 and 5.2 from previous measurements of the same kind, are already available $(j = 0,1,2,...)$. The measurements shall be carried out on different samples with differing activities, but in other respects as far as possible under similar conditions. One of the measurements can be a background effect measurement or a blank measurement with $\tilde{y} = 0$ and, for instance, $j = 0$. Then, $y_0 = 0$ shall be set and $\tilde{u}(0) = u(y_0)$. The measurement currently carried out can be taken as a further measurement with $j = 1$.

The function $\tilde{u}(\tilde{y})$ often shows a rather slow increase. Therefore, the approximation $\tilde{u}(\tilde{y}) = u(y_1)$ is sufficient in some of these cases, especially if the primary measurement result, y_1 , of the measurand is not much larger than the associated standard uncertainty $u(y_1)$.

If only $\tilde{u}(0) = u(y_0)$, $y_1 > 0$ and $u(y_1)$ are known, the following linear interpolation often suffices:

$$\tilde{u}^2(\tilde{y}) = \tilde{u}^2(0)(1 - \tilde{y}/y_1) + u^2(y_1)\tilde{y}/y_1 \tag{19}$$

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If the results y_0, y_1 and y_2 as well as the associated standard uncertainties $u(y_0)$, $u(y_1)$, and $u(y_2)$ from three measurements are available, the following bilinear interpolation can be used:

$$\tilde{u}^2(\tilde{y}) = u^2(y_0)\cdot\frac{(\tilde{y}-y_1)(\tilde{y}-y_2)}{(y_0-y_1)(y_0-y_2)} + u^2(y_1)\cdot\frac{(\tilde{y}-y_0)(\tilde{y}-y_2)}{(y_1-y_0)(y_1-y_2)} + u^2(y_2)\cdot\frac{(\tilde{y}-y_0)(\tilde{y}-y_1)}{(y_2-y_0)(y_2-y_1)} \quad (20)$$

If results from many similar measurements are given, the parabolic shape of the function $\tilde{u}^2(\tilde{y})$ can also be determined by an adjustment calculation.

6 Characteristic limits and assessments

6.1 Specifications

The probability, α, of the error of the first kind, the probability, β, of the error of the second kind and the probability, $1-\gamma$, for the confidence interval shall be specified. The choice depends on the application. A frequently cited choice is $\alpha = \beta$ and the value 0,05 for α and β. Then, $k_{1-\alpha} = k_{1-\beta} = 1{,}65$. If the value of 0,05 is chosen for γ, then $k_{1-\gamma/2} = 1{,}96$ (see Annex E).

If it is to be assessed whether or not a measurement procedure for the measurand satisfies the requirements to be fulfilled for scientific, legal or other reasons (see 6.6), a guideline value, y_r, as a value of the measurand, for instance, an activity, shall also be specified.

6.2 Decision threshold

The decision threshold, y^*, of the non-negative measurand according to 5.1, quantifying the physical effect of interest, is the value of the estimator, Y, which allows the conclusion that the physical effect is present, if the primary measurement result, y, exceeds the decision threshold, y^*. If the result, y, is below the decision threshold, y^*, the result cannot be attributed to the physical effect, nevertheless it cannot be concluded that it is absent. If the physical effect is really absent, the probability of taking the wrong decision, that the effect is present, is equal to the specified probability, α (error of the first kind; see 6.1 and 6.5).

A determined primary measurement result, y, for the non-negative measurand is only significant for the true value of the measurand to differ from zero ($\tilde{y} > 0$), if it is larger than the decision threshold

$$y^* = k_{1-\alpha}\tilde{u}(0) \quad (21)$$

6.3 Detection limit

The detection limit, $y^\#$, is the smallest true value of the measurand, for which, by applying the decision rule according to 6.2, the probability of the wrong assumption that the physical effect is absent (error of the second kind) does not exceed the specified probability, β (see 6.1).

In order to find out whether a measurement procedure is suitable for the measurement purpose, the detection limit, $y^\#$, is compared with the specified guideline value, y_r, of the measurand (see 6.1 and 6.6). The detection limit, $y^\#$, is the smallest true value of the measurand which can be detected with the measurement procedure used. It is high enough compared to the decision threshold, y^*, that the probability of the error of the second kind does not exceed β. The detection limit, $y^\#$, is obtained as the smallest solution of Equation (22):

$$y^\# = y^* + k_{1-\beta}\tilde{u}(y^\#) \quad (22)$$

where $y^\# \geqslant y^*$ always applies.

Equation (22) is an implicit equation; its right-hand side also depends on $y^{\#}$. The detection limit can be calculated by solving Equation (22) for $y^{\#}$ or, more simply, by iteration (see Figure 1). Thus, an improved approximation $\tilde{y}_{i+1}$ is obtained by repeatedly substituting an approximation $\tilde{y}_i$ for $y^{\#}$ on the right-hand side of Equation (22). This leads to Equation (23):

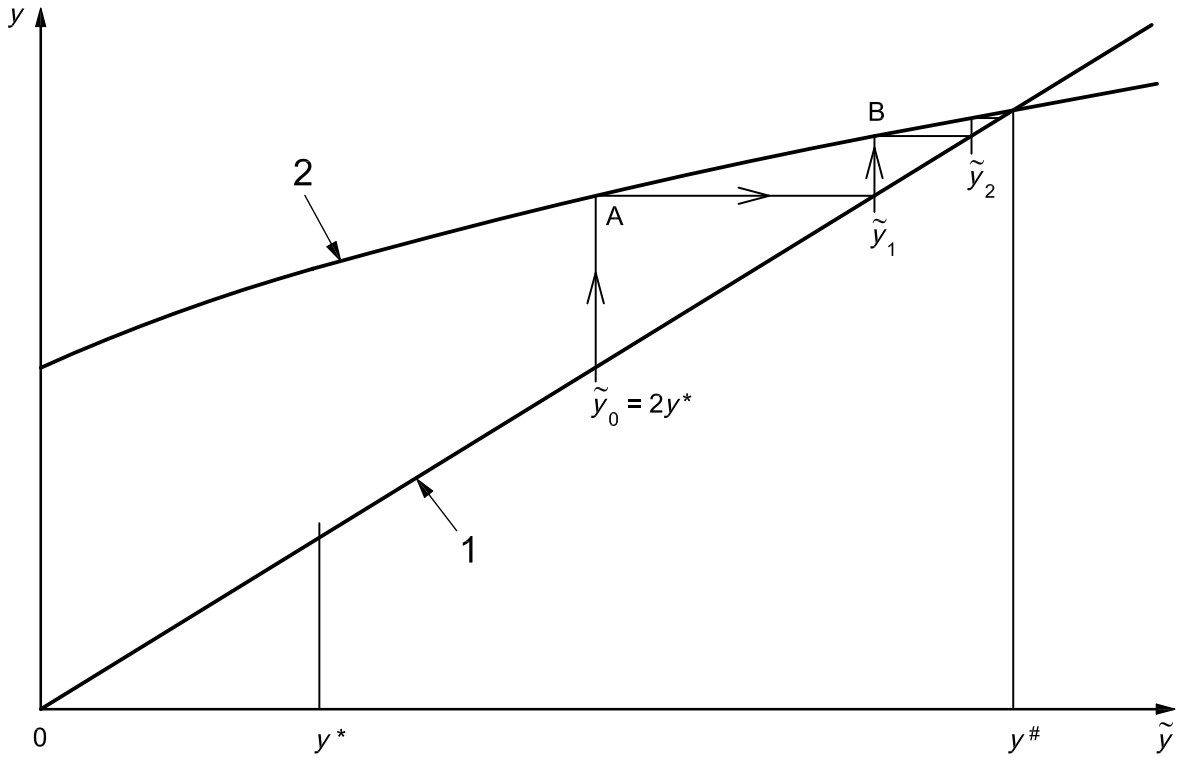
$$\tilde{y}_{i+1} = y^* + k_{1-\beta}\tilde{u}(\tilde{y}_i) \tag{23}$$

As a starting approximation, for instance, $\tilde{y}_0 = 2y^*$ can be chosen. The iteration converges in most cases, but not if Equation (22) does not have a solution, $y^{\#}$. In the latter case or if $y^{\#} < y^*$ results, a detection limit cannot be established for this measurement procedure (see 5.3.2 and 6.6). In this situation enlarging β can result in a solution to Equation (22).

After the calculation of $\tilde{y}_1$ or, for instance, with a suitable choice of e.g. $\tilde{y}_1 = 3y^*$, it is more advantageous for $i \geqslant 1$ to apply the *regula falsi*, which in general converges more rapidly. For this purpose, Equation (23) shall be replaced by

$$\tilde{y}_{i+1} = \frac{y^* + k_{1-\beta} \cdot \left[\tilde{y}_i \tilde{u}(\tilde{y}_j) - \tilde{y}_j \tilde{u}(\tilde{y}_i)\right] / (\tilde{y}_i - \tilde{y}_j)}{1 - k_{1-\beta} \cdot \left[\tilde{u}(\tilde{y}_i) - \tilde{u}(\tilde{y}_j)\right] / (\tilde{y}_i - \tilde{y}_j)} \tag{24}$$

with $j < i$. Therefore, $j = 0$ should be set or j be fixed after several iteration steps (see Figure 1).



Key

1 straight line $y = \tilde{y}$

2 curve $y = y^* + k_{1-\beta}\,\tilde{u}(\tilde{y})$

$\tilde{y}$ true value of the measurand

y estimate of the measurand

For the other symbols, see text.

Figure 1 — Calculation of the detection limit by iteration

With the iteration according to Equations (23) or (24) and beginning with a starting approximation, $\tilde{y}_0$, for instance, $\tilde{y}_0 = 2y^*$ as shown, the sequences of the improved approximations $\tilde{y}_j$ $(j = 1, 2, ...)$ converge to the detection limit $y^\#$, which is the abscissa of the intersection point of the straight line (key item 1 in Figure 1) and curve (key item 2 in Figure 1). y^* is the decision threshold. With the alternative application of the *regula falsi* according to Equation (24), the sequence, $\tilde{y}_j$, is generated by means of secants of curve 2, for instance, through points A and B. The shown hyperbolic shape of the curve (key item 2 in Figure 1) is typical of many applications, for instance, those with Equations (14) or (16). The detection limit does not exist if the curve does not intersect the straight line (key item 1 in Figure 1) at any abscissa $\tilde{y} \geqslant y^*$.

Any iteration shall be stopped if a specified accuracy of ν digits is attained, i.e. if the first digits, ν, of the successive approximations no longer change. But, if too high an accuracy is demanded, then, even with an iteration converging in principle, the successive approximations in general permanently fluctuate around and close to the exact solution but never attain it. A smaller ν shall then be chosen.

With the approximation $\tilde{u}(\tilde{y}) = u(y)$ (see 5.3.3), $y^\# = (k_{1-\alpha} + k_{1-\beta})u(y)$ applies.

The linear interpolation according to Equation (19) leads to the approximation:

$$y^\# = a + \sqrt{a^2 + (k_{1-\beta}^2 - k_{1-\alpha}^2)\,\tilde{u}^2(0)} \tag{25}$$

with

$$a = k_{1-\alpha}\,\tilde{u}(0) + \frac{1}{2}\left\{\left(k_{1-\beta}^2 \big/ y_1\right)\left[(u^2(y_1) - \tilde{u}^2(0)\right]\right\} \tag{26}$$

If $\alpha = \beta$, $y^\# = 2a$ follows.

If $\alpha = \beta$ is chosen and $\tilde{u}^2(\tilde{y})$ is obtained or approximated by a second-order polynomial $\tilde{u}^2(\tilde{y}) = c_0 + c_1\tilde{y} + c_2\tilde{y}^2$ as in Equations (14), (16) and (20), then with $k = k_{1-\alpha} = k_{1-\beta}$

$$y^* = k\sqrt{c_0} \tag{27}$$

and

$$y^\# = \frac{2y^* + k^2 c_1}{1 - k^2 c_2} \tag{28}$$

6.4 Limits of the confidence interval

The limits of the confidence interval are provided for a physical effect, recognized as present according to 6.2, in such a way that the confidence interval contains the true value of the measurand with the specified probability $1-\gamma$ (see 6.1). The limits of the confidence interval take into account the fact that the measurand is non-negative.

With a primary measurement result, y, of the measurand and the standard uncertainty, $u(y)$, associated with y (see 5.2), the lower limit of the confidence interval, $y^\triangleleft$, and the upper limit of the confidence interval, $y^\triangleright$, are provided by:

$$y^\triangleleft = y - k_p\,u(y) \text{ with } p = \omega \cdot (1 - \gamma/2) \tag{29}$$

$$y^\triangleright = y + k_q\,u(y) \text{ with } q = 1 - \omega\gamma/2 \tag{30}$$

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where

$$\omega = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{y/u(y)} \exp(-\frac{v^2}{2}) \mathrm{d}v = \Phi\left[y/u(y)\right] \tag{31}$$

For the distribution function, $\Phi(t)$, of the standardized normal distribution and for its inversion, $k_p = t$ for $\Phi(t) = p$, see Table E.1. For methods for its calculation, see Annex E or, for instance, Reference [29].

In general, the limits of the confidence interval are located neither symmetrical to y, nor to the best estimate, $\hat{y}$ (see 6.5 and Figure 2), but the probabilities of the measurand being smaller than $y^{\triangleleft}$ or larger than $y^{\triangleright}$ both equal $\gamma/2$. The relations $0 < y^{\triangleleft} < y^{\triangleright}$ apply.

$\omega = 1$ may be set if $y \geqslant 4u(y)$. In this case, the following approximations symmetrical to y apply:

$$y^{\triangleleft} = y - k_{1-\gamma/2}\, u(y) \text{ and } y^{\triangleright} = y + k_{1-\gamma/2}\, u(y) \tag{32}$$

6.5 Assessment of a measurement result

The determined primary measurement result, y, of the measurand shall be compared with the decision threshold, y^*. If $y > y^*$, the physical effect quantified by the measurand is recognized as present. Otherwise, it is decided that the effect is absent.

If $y \geqslant y^*$ and with ω according to Equation (31), the best estimate $\hat{y}$ of the measurand is given by (see 5.1 and Figure 2):

$$\hat{y} = y + \frac{u(y)\exp\left\{-y^2 \Big/ \left[2u^2(y)\right]\right\}}{\omega\sqrt{2\pi}} \tag{33}$$

The standard uncertainty associated with $\hat{y}$ reads

$$u(\hat{y}) = \sqrt{u^2(y) - (\hat{y} - y)\hat{y}} \tag{34}$$

NOTE 1 If the best estimate, $\hat{y}$, and its standard uncertainty, $u(\hat{y})$, are calculated, the recording of the primary measurement result, y, and its standard uncertainty, $u(y)$, may be omitted.

NOTE 2 If the decision rule defined by the decision threshold is not used and if $y < y^*$, the best estimate, $\hat{y}$, and its standard uncertainty, $u(\hat{y})$, can also be calculated.

The relations $y < \hat{y}$, $0 < \hat{y}$ and $y^{\triangleleft} < \hat{y} < y^{\triangleright}$ as well as $u(\hat{y}) < u(y)$ and $u(\hat{y}) < \hat{y}$ apply; moreover, for $y \geqslant 4u(y)$, the approximations

$$\hat{y} = y \;;\; u(\hat{y}) = u(y) \tag{35}$$

hold true.

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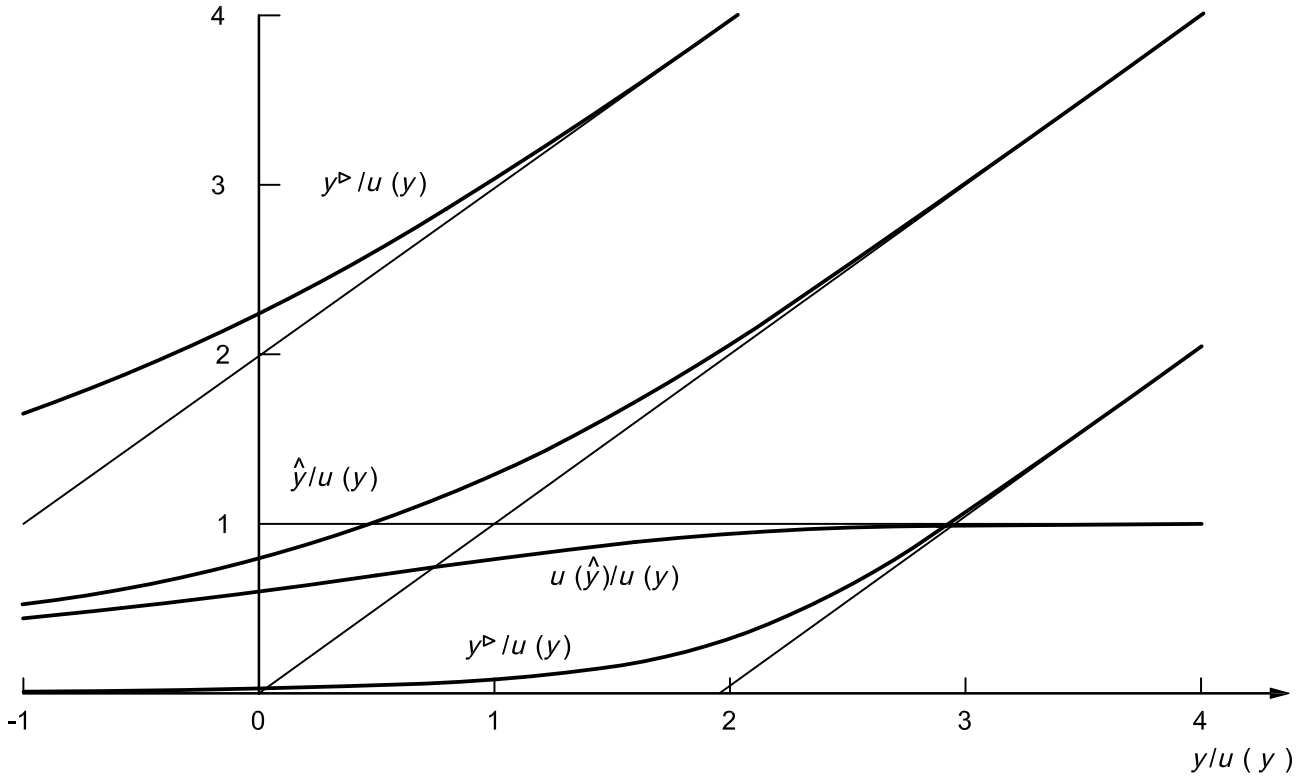

Key

$y/u(y)$ quotient of the primary measurement result of the measurand and the standard uncertainty of the measurand associated with the best estimate

For the curves, see the text.

Figure 2 — Best estimate and limits of the confidence interval

The best estimate, $\hat{y}$, of the measurand, the associated standard uncertainty, $u(\hat{y})$, the lower limit, $y^{\triangleleft}$, and the upper limit, $y^{\triangleright}$, of the confidence interval are given as functions of the primary measurement result, y. All these values are scaled with the standard uncertainty, $u(y)$, and $\gamma = 0{,}05$ is chosen. The ascending straight lines and the horizontal straight line with ordinate 1 are asymptotes.

6.6 Assessment of a measurement procedure

The decision on whether or not a measurement procedure to be applied sufficiently satisfies the requirements regarding the detection of the physical effect quantified by the measurand is made by comparing the detection limit, $y^{\#}$, with the specified guideline value, y_{r}. If $y^{\#} > y_{\mathrm{r}}$ or if Equation (22) has no solution, $y^{\#}$, the measurement procedure is not suitable for the intended measurement purpose with respect to the requirements.

To improve the situation in the case of $y^{\#} > y_{\mathrm{r}}$, it can often be sufficient to choose longer measurement durations or to preselect more counts of the measurement procedure. This reduces the detection limit.

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7 Documentation

The content of the test report depends on the specific application as well as on demands of the customer or regulator. Independently of this, information shall be retained in order to justify the data of the test report and to guarantee traceability. This applies in particular to:

a) a reference to this International Standard, i.e. ISO 11929:2009;

b) the physical effect of interest, measurand and model of the evaluation;

c) the probabilities α and β of the errors of the first and second kind, respectively, and, if necessary, the guideline value, y_r;

d) the primary measurement result, y, and the standard uncertainty, $u(y)$, associated with y;

e) the decision threshold, y^*;

f) detection limit $y^\#$;

g) if necessary, a statement as to whether or not the measurement procedure is suitable for the intended measurement purpose;

h) a statement as to whether or not the physical effect is recognized as being present;

NOTE If the physical effect is not recognized as being present, i.e. if $y < y^*$, it is occasionally demanded by the regulator to document $< y^\#$ instead of the measured result, y. Such documentation can be meaningful since it allows, by comparison with the guideline value, to demonstrate that the measurement procedure is suitable for the intended measurement purpose.

i) in addition, if the physical effect is recognized as being present, the lower limit of the confidence interval, $y^\triangleleft$, and the upper limit of the confidence interval, $y^\triangleright$, with the probability, $1-\gamma$, for the confidence interval, best estimate, $\hat{y}$, of the measurand, and standard uncertainty, $u(\hat{y})$ associated with $\hat{y}$.

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Annex A
(informative)

Overview of the general procedure

A.1 Introduction of the model

Introduction of the non-negative measurand, Y, and of its representation as a function of the input quantities, X_i (model; X_1 is the gross effect; see 5.1 and 5.2.1):

$$Y = G(X_1, ..., X_m) \tag{A.1}$$

A.2 Preparation of the input data and specifications

Determination of the estimates, x_i, of the input quantities, X_i, with the associated standard uncertainties, $u(x_i)$, in conformity with ISO/IEC Guide 98-3 (see References [1, 2]), from measurements and previous investigations. For a count rate, $X_i = \rho_i$, with the counting result, n_i, obtained from a measurement of duration, t_i, introduce $x_i = n_i/t_i$ and $u^2(x_i) = n_i/t_i^2$ (see 5.2.1). In particular, $u(x_1) = h_1(x_1) = \sqrt{x_1/t_1}$ applies for the gross effect, X_1 (see 5.3.1 and A.4).

Specifications: probabilities α, β and γ, and the guideline value, y_r (see 6.1).

A.3 Calculation of the primary measurement result, y, with the associated standard uncertainty, $u(y)$

$$y = G(x_1, ..., x_m) \tag{A.2}$$

$$u^2(y) = \sum_{i=1}^{m} \left(\frac{\partial G}{\partial X_i} \right)^2 u^2(x_i) \tag{A.3}$$

for presupposed uncorrelated input quantities, X_i (see 5.2.1 and A.2). Otherwise, see the references in A.2. The estimates, x_1, ..., x_m, shall be substituted in $\partial G/\partial X_i$.

A.4 Calculation of the standard uncertainty, $\tilde{u}(\tilde{y})$

If $u(x_1)$ is known as a function $h_1(x_1)$, y is replaced by $\tilde{y}$ and Equation (A.2) is solved for x_1. With $\tilde{y}$ specified, x_1 can also be numerically calculated from Equation (A.2), for instance by means of an iteration procedure. This results in x_1 as a function of $\tilde{y}$ and x_2, ..., x_m. The function replaces x_1 in Equation (A.3) and in $h_1(x_1)$. This yields $\tilde{u}(\tilde{y})$ instead of $u(y)$ (see 5.3.2). Otherwise, $\tilde{u}(\tilde{y})$ follows as an approximation by interpolating the data y and $u(y)$ from several measurements (see 5.3.3).

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A.5 Calculation of the decision threshold, y^*

$$y^* = k_{1-\alpha}\,\tilde{u}(0) \tag{A.4}$$

See 6.2. Assessment: an effect of the measurand, Y, is recognized as present if $y > y^*$ (see 6.5). If not, A.7 and A.8 are omitted.

A.6 Calculation of the detection limit, $y^\#$

The detection limit, $y^\#$, is the smallest solution of Equation (A.5):

$$y^\# = y^* + k_{1-\beta}\,\tilde{u}(y^\#) \tag{A.5}$$

It can be calculated by iteration with the starting approximation $y^\# = 2y^*$ (see 6.3). Assessment: the measurement procedure is not suitable for the measurement purpose if $y^\# > y_r$ or if $y^\#$ does not exist (see 6.6).

A.7 Calculation of the limits of the confidence interval, $y^\triangleleft$ and $y^\triangleright$

$$y^\triangleleft = y - k_p\,u(y) \text{ with } p = \omega\cdot(1-\gamma/2);\ y^\triangleright = y + k_q\,u(y) \text{ with } q = 1-\omega\gamma/2 \tag{A.6}$$

where $\omega = \Phi\left[y/u(y)\right]$ (see 6.4; for the calculation of ω, k_p and k_q, see Annex E).

A.8 Calculation of the best estimate, $\hat{y}$, of the measurand with the associated standard uncertainty, $u(\hat{y})$

$$\hat{y} = y + \frac{u(y)\exp\left\{-y^2\Big/\left[2u^2(y)\right]\right\}}{\omega\sqrt{2\pi}};\ u(\hat{y}) = \sqrt{u^2(y) - (\hat{y}-y)\,\hat{y}} \tag{A.7}$$

See 6.5.

A.9 Preparation of the documentation

The report of the results is according to Clause 7.

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Annex B
(normative)

Various applications

B.1 General aspects

The procedure described in the main part of this International Standard is so general that it allows a large variety of applications to similar measurements. Some important cases are discussed in the following clauses. They do not differ in their models from those in the main part, but merely in the interpretation of the input quantities, X_1 and X_2, and in setting up the corresponding estimates, x_1 and x_2, and standard uncertainties, $u(x_1)$ and $u(x_2)$.

With each of the following applications dealt with in Annexes B and C, the respective main task consists of determining the primary measurement result, y, of the measurand and the associated standard uncertainty, $u(y)$, according to 5.2 or A.3 as well as the standard uncertainty, $\tilde{u}(\tilde{y})$, as a function of the measurand according to 5.3 or A.4. Subsequently, with all applications, the decision threshold, y^*, the detection limit, $y^\#$, the limits, $y^\triangleleft$ and $y^\triangleright$, of the confidence interval, as well as the best estimate, $\hat{y}$, of the measurand with the associated standard uncertainty, $u(\hat{y})$, shall be calculated in the same way according to Clause 6 or A.5 to A.8. This is no longer pointed out in the following clauses. Numerical examples of the applications are discussed in Annex D.

B.2 Counting measurements on moving objects

Let a counting measurement be carried out by moving the measurement object along a specified measurement distance on a straight line passing a radiation detector (or vice versa). Data obtained from the measurement during this travel are, on the one hand, the counted numbers, n_g or n_0, of the recorded pulses and, on the other hand, the measurement durations, t_g or t_0, respectively. In general, the measurement durations can be determined with negligible measurement uncertainties compared to all other measurement uncertainties that shall be taken into account. Therefore, they can be taken as constants and the measurement as a measurement with time preselection.

The reduction of the background count rate by the shielding effect of the measurement object can be taken into account by means of the shielding factor, f, by setting $X_3 = f$ and $X_4 = 0$ in Equation (4). f can be obtained experimentally from previous measurements as an arithmetic mean value and the standard uncertainty, $u(f)$, associated with f, as the empirical standard deviation of the arithmetic mean value. They can alternatively be obtained as the expectation value and the standard deviation, $u(f) = \Delta f / \sqrt{12}$, respectively, from a rectangular distribution with the width Δf over the region of the possible values of f.

In the simplest case where the model shall be specified in the form of $Y = X_1 - X_2 X_3 = \rho_g - \rho_0 f$ and where the measurement durations, t_g and t_0, are preselected and the estimates, $x_1 = n_g / t_g = r_g$ and $x_2 = n_0 / t_0 = r_0$, with the associated squared standard uncertainties, $u^2(x_1) = r_g / t_g$ and $u^2(x_2) = r_0 / t_0$, are applied, the results read

$$y = \frac{n_g}{t_g} - \frac{n_0}{t_0} f = r_g - r_0 f \; ; \; u(y) = \sqrt{\frac{r_g}{t_g} + \frac{r_0}{t_0} f^2 + r_0^2 u^2(f)} \tag{B.1}$$

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Replacing y by $\tilde{y}$ and eliminating $r_g = \tilde{y} + r_0 f$, because of $u^2(x_1) = h_1^2(x_1) = x_1/t_g = r_g/t_g$, yields

$$\tilde{u}(\tilde{y}) = \sqrt{\frac{\tilde{y} + r_0 f}{t_g} + \frac{r_0}{t_0} f^2 + r_0^2 u^2(f)} \tag{B.2}$$

B.3 Measurements with ratemeters

A ratemeter records the rate of pulses arriving at the input of the meter. Here, a ratemeter is understood as a linear, analogously working count rate measuring instrument where the output signal increases sharply (with a negligible rise time constant) upon the arrival of an input pulse and then decreases exponentially with a relaxation time constant, τ, until the next input pulse arrives. The signal increase shall be the same for all pulses and the relaxation time constant shall be independent of the count rate. A digitally working count rate measuring instrument simulating the one just described is also taken as a ratemeter having to be considered here.

Each particular measurement using a ratemeter shall be carried out in the stationary state of the ratemeter. This requires at least a sufficiently large fixed time span between the start of measurement and reading the ratemeter indication. This applies to each sample and to each background effect measurement. According to Reference [30], fixed time spans of 3τ or 7τ correspond to deviations of the indication by 5 % or 0,1 % of the magnitude of the difference between the indication at the start of measurement and that at the end of the time span. If further uncertain influences have to be taken into account, a time span of 7τ should be chosen, if possible.

The expectation values, ρ_g and ρ_0, of the output signals of the ratemeter in the cases of measuring the gross and background effects, respectively, are taken as the input quantities, X_1 and X_2, for the calculation of the characteristic limits: $X_1 = \rho_g$ and $X_2 = \rho_0$. With the values r_g and r_0 of the output signals determined at the respective moments of measurement, the following approaches result for the values of the input quantities and the associated standard uncertainties:

$$x_1 = r_g \; ; \quad x_2 = r_0 \tag{B.3}$$

$$u^2(x_1) = \frac{r_g}{2\tau_g} \; ; \quad u^2(x_2) = \frac{r_0}{2\tau_0} \tag{B.4}$$

In Equation (B.4), approximations with a maximum relative deviation of 5 % for $r_g \cdot \tau_g \geqslant 0{,}65$ and of 1 % for $r_g \cdot \tau_g \geqslant 1{,}32$ are specified according to Reference [30]. The same applies to $r_0 \cdot \tau_0$. The relaxation time constants, τ_g and τ_0, shall be adjusted to fulfil requirements regarding the maximum relative deviations.

The ratemeter measurement is equivalent to a counting measurement with time preselection according to 5.3.2 and with the measurement durations, $t_g = 2\tau_g$ and $t_0 = 2\tau_0$. The quotients n_g/t_g and n_0/t_0 of the counting measurement shall be replaced here by the measured count rate values, r_g and r_0, respectively, of the ratemeter measurement. This applies, in particular, to Equation (13). See also the numerical example in D.2.2. The standard uncertainties of the relaxation time constants do not appear in the equations and are therefore not needed.

In the simplest case where the model shall be specified in the form of $Y = X_1 - X_2 = \rho_g - \rho_0$, Equations (B.3) and (B.4) lead to

$$y = r_g - r_0 \; ; \quad u(y) = \sqrt{\frac{r_g}{2\tau_g} + \frac{r_0}{2\tau_0}} \tag{B.5}$$

Replacing y by $\tilde{y}$ and eliminating $r_g = \tilde{y} + r_0$, because of $u^2(x_1) = h_1^2(x_1) = x_1/(2\tau_g) = r_g/(2\tau_g)$, yields

$$\tilde{u}(\tilde{y}) = \sqrt{\frac{\tilde{y} + r_0}{2\tau_g} + \frac{r_0}{2\tau_0}} \tag{B.6}$$

B.4 Repeated counting measurements with random influences

B.4.1 General aspects

Random influences due to, for instance, sample treatment and instruments cause measurement deviations, which can be different from sample to sample. In such cases, the counting results, n_i, of the counting measurements on several samples of a radioactive material to be examined, on several blanks of a radioactively labelled blank material, and on several reference samples of a standard reference material are therefore respectively averaged to obtain suitable estimates, x_1 and x_2, of the input quantities, X_1 and X_2, and the associated standard uncertainties, $u(x_1)$ and $u(x_2)$, respectively. Accordingly, X_1 shall be considered as the mean gross count rate and X_2 as the mean background count rate. Therefore, the measurand, Y, with the sought-after true value, $\tilde{y}$, shall also be taken as an averaged quantity, for instance as the mean net count rate or mean activity of the samples. In this annex, all symbols belonging to the countings on the samples, blanks and reference samples are marked by the subscripts g, 0 and r, respectively. In each case, arithmetic averaging over m countings of the same kind carried out with the same preselected measurement duration, t (time preselection), is denoted by an overline. For m counting results, n_i ($i = 1, ..., m$; $m > 1$), which are obtained in such a way and shall be averaged, the mean value, $\overline{n}$, and the empirical variance, s^2, of the values, n_i, are given by

$$\overline{n} = \frac{1}{m}\sum_{i=1}^{m} n_i \;\; ; \;\; s^2 = \frac{1}{m-1}\sum_{i=1}^{m}(n_i - \overline{n})^2 \tag{B.7}$$

The procedures in B.4.2 and B.4.3 are approximations for sufficiently large counting results $n_i >> 1$ and $\overline{n} << s^2$, which allow the random influences to be recognized in addition to those of the Poisson statistics [see Equation (B.12)].

A numerical example of a measurement with random influences is described in D.3.

B.4.2 Procedure with unknown influences

In the case of unknown influences, the following expressions are valid for the mean gross count rate, X_1, and the mean background count rate, X_2:

$$x_1 = \overline{n}_g/t_g \;\; ; \;\; x_2 = \overline{n}_0/t_0 \tag{B.8}$$

$$u^2(x_1) = s_g^2/(m_g t_g^2) \;\; ; \;\; u^2(x_2) = s_0^2/(m_0 t_0^2) \tag{B.9}$$

With the approaches according to Equations (B.8) and (B.9), Equations (6) and (9) yield

$$y = \left(\frac{\overline{n}_g}{t_g} - \frac{\overline{n}_0}{t_0}x_3 - x_4\right)\cdot w \tag{B.10}$$

$$u(y) = \sqrt{w^2 \cdot \left[s_g^2/(m_g t_g^2) + x_3^2 s_0^2/(m_0 t_0^2) + (\overline{n}_0/t_0)^2 \cdot u^2(x_3) + u^2(x_4)\right] + y^2 u_{rel}^2(w)} \tag{B.11}$$

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$u^2(x_1)$ is not given as a function $h_1^2(x_1)$ of x_1. Therefore, $\tilde{u}^2(\tilde{y})$ shall be determined as an approximation according to 5.3.3, for instance, according to Equation (19), where the current result, y, can be used as y_1. For this purpose and for the calculation of $\tilde{u}^2(0)$, i.e. for $\tilde{y} = 0$, the missing s_g^2/t_g^2 shall be replaced by s_0^2/t_0^2, since both these values are then variance estimates of the same distribution of count rate values, independent of t_g, t_0, m_g and m_0.

B.4.3 Procedure with known influences

Another procedure, appropriate when small random influences are present, is based on the approach

$$s^2 = \overline{n} + \vartheta^2 \overline{n}^2 \tag{B.12}$$

The first term, $\overline{n}$, of Equation (B.12) corresponds to the numbers n_i of pulses according to the Poisson law in the absence of random influences. These influences are described by the second term, $\vartheta^2\overline{n}^2$, assuming an empirical relative standard deviation, ϑ, valid for all samples and countings and caused by these influences. This influence parameter, ϑ, can be calculated from the data of counting measurements of the reference samples by combining Equation (B.12) with Equation (B.7):

$$\vartheta^2 = (s_r^2 - \overline{n}_r)/\overline{n}_r^2 \tag{B.13}$$

Instead of the data from counting measurements of the reference samples, those for other samples can be used which were previously examined, not explicitly for reference purposes but under conditions similar to those of the reference samples.

If $\vartheta^2 < 0$ results, the approach and the data are not compatible. The number, m_r, of the reference samples should then be enlarged or $\vartheta = 0$ be set. Moreover, $\vartheta < 0{,}2$ should be obtained. Otherwise, one can proceed according to B.4.2.

Instead of Equation (B.9), the expressions

$$u^2(x_1) = (\overline{n}_g + \vartheta^2\overline{n}_g^2)/(m_g t_g^2)\ ;\quad u^2(x_2) = (\overline{n}_0 + \vartheta^2\overline{n}_0^2)/(m_0 t_0^2) \tag{B.14}$$

now apply with Equation (B.12). The cases $m_g = 1$ and $m_0 = 1$ are permitted here. Therefore, with $x_1 = \overline{n}_g / t_g$ and Equation (B.14), $u^2(x_1)$ is given as a function of x_1 by:

$$u^2(x_1) = h_1^2(x_1) = (x_1/t_g + \vartheta^2 x_1^2)/m_g \tag{B.15}$$

Equations (B.8) and (B.10) remain valid for $x_3 = 1$ with $u(x_3) = 0$ and $x_4 = 0$ with $u(x_4) = 0$. Furthermore, according to Equation (9), it follows that:

$$u(y) = \sqrt{w^2 \cdot \left[u^2(x_1) + u^2(x_2)\right] + y^2 u_{rel}^2(w)} \tag{B.16}$$

$u^2(x_1)$ and $u^2(x_2)$ according to Equation (B.14) shall be inserted.

In order to calculate $\tilde{u}(\tilde{y})$, the result, y, is replaced by $\tilde{y}$ and Equation (B.10) is solved for $x_1 = \overline{n}_g/t_g$. This yields $x_1 = \tilde{y}/w + \overline{n}_0/t_0$. The estimate, x_1, determined in this way in the current case, shall be substituted in Equation (B.15) and $u^2(x_1)$ obtained therefrom in Equation (B.16). This finally leads to $\tilde{u}(\tilde{y})$ (see also 5.3):

$$\tilde{u}(\tilde{y}) = \sqrt{\tilde{y}^2\left[\frac{\vartheta^2}{m_g} + u_{rel}^2(w)\right] + \frac{\tilde{y}w}{m_g}\left(\frac{2\overline{n}_0\vartheta^2}{t_0} + \frac{1}{t_g}\right) + w^2\left(\frac{\overline{n}_0}{m_g t_0 t_g} + \frac{\overline{n}_0^2\vartheta^2}{m_g t_0^2} + \frac{\overline{n}_0 + \vartheta^2\overline{n}_0^2}{m_0 t_0^2}\right)} \tag{B.17}$$

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The condition according to Equation (17) shall be replaced here by the condition

$$k_{1-\beta} \cdot \sqrt{\frac{\vartheta^2}{m_g} + u_{rel}^2(w)} < 1 \qquad \text{(B.18)}$$

B.5 Counting measurements on filters during accumulation of radioactive material

B.5.1 General aspects

For monitoring flowing fluid media (gas or liquid, for instance vent air or room air in nuclear installations or water), a counting measurement can be continuously carried out on a filter during the accumulation of radioactive material from the medium. The measurement consists of a temporal sequence of consecutive measurement intervals of the same duration, t. The half-lives of the nuclides accumulated on the filter are assumed to be long compared to the total duration of all measurement intervals, the data of which are used in the following calculation of the characteristic limits. In addition, the background effect is assumed to remain constant during the whole measurement. There are two measurands, Y, of interest:

a) the activity concentration, $A_{V,j}$ (activity divided by the total volume of the sample, see ISO 31-9), of the radioactive nuclides entrained by the medium, accumulated on the filter and measured during the measurement interval, j, of duration, t [case a), see B.5.2];

b) the change, $\Delta A_{V,j}$, in the activity concentration according to case a), compared with the mean activity concentration, $\overline{A}_{V,j}$, from m preceding measurement intervals [case b), see B.5.3].

It is sufficient for cases a) and b) to introduce the respective models according to 5.2 that describe the measurands, $Y = A_{V,j}$ and $Y = \Delta A_{V,j}$, as functions of the input quantities, X_i, and to specify the estimates, x_i, with the associated standard uncertainties, $u(x_i)$, of the input quantities, X_i. Everything else then follows according to 5.2.2, 5.3.2 and Clause 6 and analogously to B.2 and B.3. A numerical example is described in D.4.

The activity is divided by the sample volume, i.e. by the volume, V, of the medium flowing through the filter during the measurement of duration, t. This volume, V, with the associated standard uncertainty, $u(V)$, as well as a calibration factor, ε, which shall be considered with the associated standard uncertainty, $u(\varepsilon)$, are assumed to be known from previous investigations. The efficiency of the filter is assumed to be contained in ε. The standard uncertainty, $u(t)$, of the measurement duration, t, is neglected since t can be measured far more exactly than all the other quantities involved and can thus be taken as a constant.

B.5.2 Activity concentration as the measurand

In case a), $Y = A_{V,j}$ is the measurand of the measurement interval, j. The input quantities, X_i, are specified as follows: $X_1 = \rho_j$, $X_2 = \rho_{j-1}$, $X_5 = \varepsilon$ and $X_7 = V$, where ρ_j is the gross count rate in the measurement interval j. There are no further input quantities, they are set constant equalling 0 for X_4 and 1 otherwise with zero uncertainties. The model according to Equation (4) now reads

$$Y = A_{V,j} = \frac{X_1 - X_2}{X_5 X_7} = \frac{\rho_j - \rho_{j-1}}{\varepsilon V} \qquad \text{(B.19)}$$

Because of the background effect assumed to be constant, its contributions cancel out in the difference.

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Similar to 5.2.2, the estimates, x_1 and x_2, with the associated standard uncertainties, $u(x_1)$ and $u(x_2)$, of the input quantities, X_1 and X_2, respectively, are specified as follows, with n_j being the number of events recorded in the measurement interval j:

$$x_1 = r_j = n_j/t \;;\quad u^2(x_1) = r_j/t \tag{B.20}$$

$$x_2 = r_{j-1} = n_{j-1}/t \;;\quad u^2(x_2) = r_{j-1}/t \tag{B.21}$$

Obviously, $u(x_1)$ is thus known as a function $h_1(x_1)$ of x_1, which is needed for the decision threshold and the detection limit, since:

$$u(x_1) = \sqrt{r_j/t} = h_1(x_1) = \sqrt{x_1/t} \tag{B.22}$$

With the preceding approaches and $w = 1/(\varepsilon V)$ with $u^2_{\text{rel}}(w) = u^2(\varepsilon)/\varepsilon^2 + u^2(V)/V^2$, the following is obtained according to 5.2.2 and 5.3.2:

$$y = \frac{x_1 - x_2}{x_5 x_7} = \frac{r_j - r_{j-1}}{\varepsilon V} \tag{B.23}$$

$$\begin{aligned} u(y) &= \sqrt{w^2 \cdot \left[u^2(x_1) + u^2(x_2)\right] + y^2 u^2_{\text{rel}}(w)} \\ &= \frac{1}{\varepsilon V}\sqrt{\frac{r_j + r_{j-1}}{t} + (r_j - r_{j-1})^2\left[\frac{u^2(\varepsilon)}{\varepsilon^2} + \frac{u^2(V)}{V^2}\right]} \end{aligned} \tag{B.24}$$

Replacing y with $\tilde{y}$ yields with Equations (B.24) and (12)

$$x_1 = r_j = \tilde{y}/w + x_2 = \tilde{y}\varepsilon V + r_{j-1} \tag{B.25}$$

$$\begin{aligned} \tilde{u}(\tilde{y}) &= \sqrt{w^2 \cdot \left[h_1^2(\tilde{y}/w + x_2) + u^2(x_2)\right] + \tilde{y}^2 u^2_{\text{rel}}(w)} \\ &= \sqrt{\frac{(\tilde{y}\varepsilon V + x_2)/t + u^2(x_2)}{(\varepsilon V)^2} + \tilde{y}^2 \cdot \left[\frac{u^2(\varepsilon)}{\varepsilon^2} + \frac{u^2(V)}{V^2}\right]} \\ &= \sqrt{\frac{\tilde{y}\varepsilon V + 2r_{j-1}}{(\varepsilon V)^2 t} + \tilde{y}^2 \cdot \left[\frac{u^2(\varepsilon)}{\varepsilon^2} + \frac{u^2(V)}{V^2}\right]} \end{aligned} \tag{B.26}$$

B.5.3 Change in the activity concentration as the measurand

Case b) only differs from case a) discussed in B.5.2 by a different definition of X_2. The model reads:

$$\begin{aligned} Y = \Delta A_{V,j} &= A_{V,j} - \overline{A}_{V,j} = \frac{X_1 - X_2}{X_5 X_7} \\ &= \frac{1}{\varepsilon V}\left[\rho_j - \rho_{j-1} - \frac{1}{m}\sum_{k=1}^{m}(\rho_{j-k} - \rho_{j-k-1})\right] = \frac{1}{\varepsilon V}\left[\rho_j - (1 + \frac{1}{m})\rho_{j-1} + \frac{1}{m}\rho_{j-m-1}\right] \end{aligned} \tag{B.27}$$

Instead of $X_2 = \rho_{j-1}$, now

$$X_2 = \left(1 + \frac{1}{m}\right)\rho_{j-1} - \frac{1}{m}\,\rho_{j-m-1} \tag{B.28}$$

is valid with $X_1 = \rho_j$. Hence it follows

$$x_2 = \left(1 + \frac{1}{m}\right) r_{j-1} - \frac{1}{m} r_{j-m-1}\,; \quad u^2(x_2) = \left(1 + \frac{1}{m}\right)^2 \frac{r_{j-1}}{t} + \frac{r_{j-m-1}}{m^2 t} \tag{B.29}$$

The values x_2 and $u^2(x_2)$, calculated according to Equation (B.29), shall be substituted in Equations (B.23) to (B.26) to obtain y, $u(y)$ and $\tilde{u}(\tilde{y})$.

The model according to Equation (B.27) applies to the test for an increase in the activity concentration. If a decrease is to be examined, $Y = \overline{A}_{V,j} - A_{V,j}$ shall be specified as the measurand, i.e. X_1 and X_2 shall be interchanged so that the measurand becomes non-negative as demanded.

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Annex C
(normative)

Applications to counting spectrometric measurements

C.1 General aspects

This International Standard can also be applied to counting spectrometric measurements when a particular line in a measured multi-channel spectrum should be considered and no adjustment calculations, for instance, an unfolding, have to be carried out. The net intensity of the line is first determined according to C.1 to C.3 by separating the background. Then, if another measurand, for instance, an activity, shall be calculated, proceed according to 5.2 and 5.3 (see C.4). The background in spectrometric measurements is understood as the number of events of no interest in the region of a regarded line in the spectrum. The events can be due both to the background effect by the environmental radiation and also to the sample itself (for instance, from other lines).

Independent, Poisson-distributed random variables, N_i ($i = 1, ..., m$ as well as $i = \mathrm{g}$), are assigned to selected channels of a measured multi-channel spectrum with the contents, n_i, of the channels (or channel regions), and the expectation values of the N_i are taken as input quantities, X_i (see F.1). If necessary, the channels of a channel region of the spectrum can be combined to form a single channel. In this annex, ϑ_i is the lower and ϑ_i' is the upper limit of channel i; ϑ is, for instance, the energy or time or another continuous scaling variable assigned to the channel number. The channel widths, $t_i = \vartheta_i' - \vartheta_i$, correspond to t according to F.1. Thus, $X_i = \rho_i t_i$ with the mean spectral density, ρ_i, in channel i, and $x_i = n_i$ is an estimate of X_i with the standard uncertainty, $u(x_i) = \sqrt{n_i}$, associated with x_i . For $i = \mathrm{g}$, the quantities, n_g and $X_\mathrm{g} = \rho_\mathrm{g} t_\mathrm{g}$, represent the combined channels of a line of interest in the spectrum. The measurand, Y , with the true value, $\tilde{y}$, is the net intensity of the line, i.e. the expectation value of the net content of channel, $i = \mathrm{g}$ (region B, see C.2). (For the appropriate determination of channel regions, see C.3.)

At first, the background of the line of interest shall be determined, which also includes the contributions of the tails of disturbing lines. A suitable function, $H(\vartheta; a_1, ..., a_m)$, representing the spectral density of the line background with the parameters a_k , is introduced so that:

$$n_i = \int_{\vartheta_i}^{\vartheta_i'} H(\vartheta; a_1, ..., a_m)\,\mathrm{d}\vartheta \; ; \quad (i = 1, ..., m) \tag{C.1}$$

from which the a_k shall be calculated as functions of the n_i .The background contribution to the line is therefore:

$$z_0 = \int_{\vartheta_\mathrm{g}}^{\vartheta_\mathrm{g}'} H(\vartheta; a_1, ..., a_m)\,\mathrm{d}\vartheta \tag{C.2}$$

The random variable, Z_0 , associated with the background contribution, z_0 , implicitly is a function of the input quantities, X_i , because z_0 is calculated from the $x_i = n_i$. The model approach for the measurand, Y, reads:

$$Y = G(X_\mathrm{g}, X_1, ..., X_m) = X_\mathrm{g} - Z_0 \tag{C.3}$$

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and leads to:

$$y = n_g - z_0 \;;\quad u^2(y) = n_g + u^2(z_0) \;;\quad u^2(z_0) = \sum_{i=1}^{m}\left(\sum_{k=1}^{m}\frac{\partial z_0}{\partial a_k}\frac{\partial a_k}{\partial n_i}\right)^2 n_i \tag{C.4}$$

The bracketed sum equals $\partial z_0/\partial n_i$. For the calculation of the function $\tilde{u}^2(\tilde{y})$, the net content, $\tilde{y}$, of channel g is first specified. Then, y in Equation (C.4) is replaced with $\tilde{y}$. This allows n_g to be eliminated, which is not available if $\tilde{y}$ is specified. This results in $n_g = \tilde{y} + z_0$ and:

$$\tilde{u}^2(\tilde{y}) = \tilde{y} + z_0 + u^2(z_0) \tag{C.5}$$

The characteristic limits according to Clause 6 then follow from Equations (C.4) and (C.5).

If the approach, linear in the a_k:

$$H(\vartheta) = \sum_{k=1}^{m} a_k \psi_k(\vartheta) \tag{C.6}$$

is applied with given functions $\psi_k(\vartheta)$, Equation (C.1) represents a system of linear equations for the a_k. Thus, the a_k depend linearly on the n_i and the partial derivatives in Equation (C.4) do not depend on the n_i. From this,

$$u^2(z_0) = \sum_{i=1}^{m} b_i^2 n_i \tag{C.7}$$

with quantities, b_i, not depending on the n_i. Equation (C.7) also follows when the background contribution, z_0, to the line is calculated linearly from the channel contents, n_i, with suitably specified coefficients, b_i:

$$z_0 = \sum_{i=1}^{m} b_i n_i \tag{C.8}$$

C.2 Application according to the background shape

If events of a single line with a known location in the spectrum are to be detected, the following cases of the background shape as a function of ϑ and the associated approaches shall be distinguished.

a) Constant background: approach $H(\vartheta) = a_1$ (constant, $m = 1$).

b) Linear background, which can often be assumed with gamma radiation: approach $H(\vartheta) = a_1 + a_2\vartheta$ (straight line, $m = 2$).

c) Weakly curved background with disturbing neighbouring lines: approach $H(\vartheta) = a_1 + a_2\vartheta + a_3\vartheta^2 + a_4\vartheta^3$ (cubic parabola, $m = 4$).

d) Strongly curved background, which can be present with strongly overlapping lines, for instance with alpha radiation: approach according to Equation (C.6).

In cases a), b) and c), the scaling variable, ϑ, is required to be linearly assigned to the channel number.

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In cases a) and b), it is suitable for the background determination to introduce three adjacent channel regions, A_1, B and A_2, in the following way.

Region B comprises all the channels belonging to the line and has the total content, n_g, and the width, t_g. If the line shape can be assumed as a Gaussian curve with the full width, h, at half-maximum, region B shall be placed as symmetrically as possible over the line. If fluctuations of the channel assignment cannot be excluded or the background does not dominate, for instance, with pronounced lines, the following should be chosen:

$$t_g \approx 2{,}5\,h \tag{C.9}$$

In case of a dominant background, the most favourable width:

$$t_g \approx 1{,}2\,h \tag{C.10}$$

shall be specified for region B. This region then covers approximately the portion $f = 0{,}84$ of the line area (see also C.4). In general, $f = 2\Phi(v\sqrt{2\ln 2}) - 1$, if $t_g = vh$ with a chosen factor v.

In principle, the full width h at half-maximum shall be determined from the resolution of the measuring system or under the same measurement conditions by means of a reference sample emitting the line to be investigated strongly enough, or from neighbouring lines with comparable shapes and widths. Region B shall comprise an integer number of channels, so that t_g is rounded up accordingly.

Regions A_1 and A_2, bordering region B below and above, shall be specified with the same widths, $t = t_1 = t_2$, in case b) only. The total width, $t_0 = t_1 + t_2 = 2t$, shall be chosen as large as possible, but at most so large that the background shape over all regions can still be taken as approximately constant [case a)] or linear [case b)]. n_1 and n_2 are the total contents of all channels of regions A_1 and A_2, respectively. Moreover, $n_0 = n_1 + n_2$.

Hence it follows for cases a) and b):

$$z_0 = c_0 n_0 \;;\quad u^2(z_0) = c_0^2 n_0 \;;\quad c_0 = t_g / t_0 \tag{C.11}$$

$\tilde{u}^2(\tilde{y})$ follows from Equation (C.5).

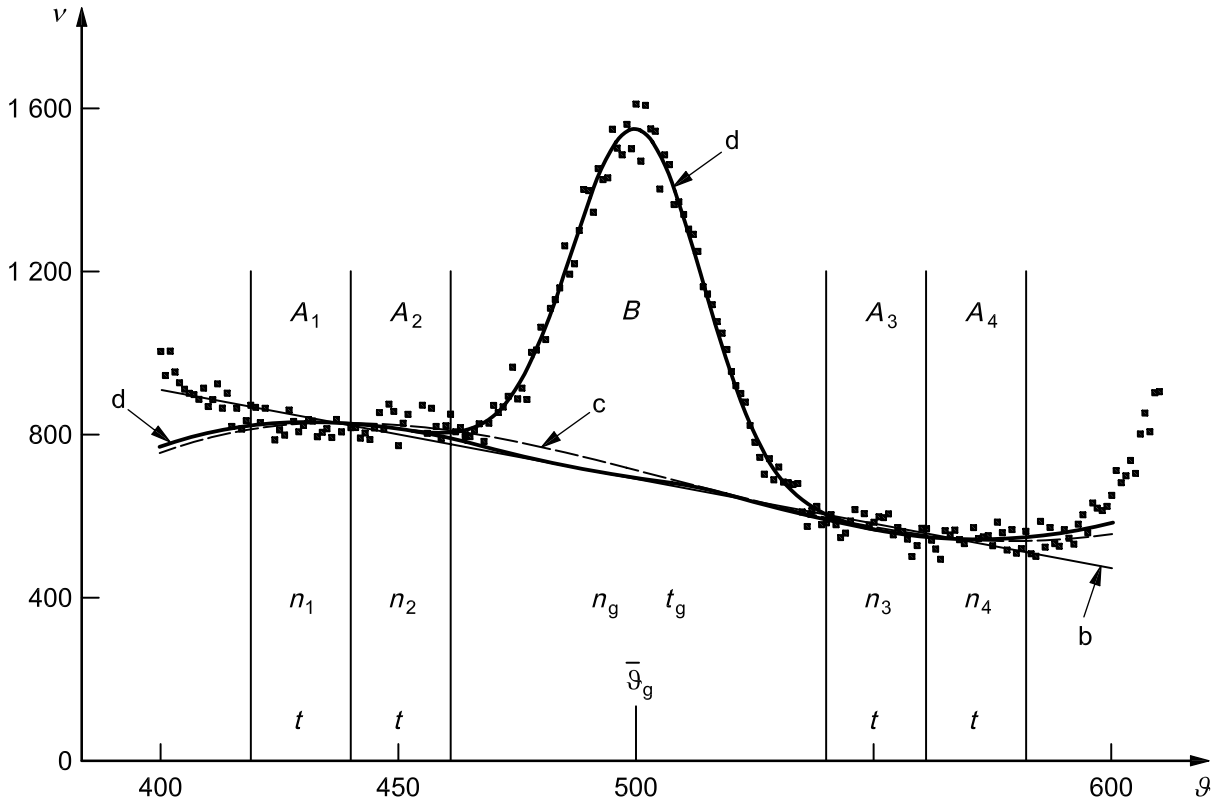
Instead, in case c), five adjacent channel regions, A_1, A_2, B, A_3 and A_4 shall be introduced in the way described above with the same widths, t, of the regions A_i (see Figure C.1). With the sum $n_0 = n_1 + n_2 + n_3 + n_4$, i.e. the total content of all channels of regions A_i, with their total width $t_0 = 4t$, and with the auxiliary quantity $n_0' = n_1 - n_2 - n_3 + n_4$, the following is then valid:

$$\begin{aligned} &z_0 = c_0 n_0 - c_1 n_0' \;;\quad u^2(z_0) = (c_0^2 + c_1^2) n_0 - 2c_0 c_1 n_0' \;; \\ &c_0 = t_g / t_0 \;;\quad c_1 = c_0 \cdot (4/3 + 4c_0 + 8c_0^2/3) / (1 + 2c_0) \end{aligned} \tag{C.12}$$

and $\tilde{u}^2(\tilde{y})$ follows from Equation (C.5). Two numerical examples of case c) are discussed in D.5.

In case d), m adjacent regions, A_i, shall be introduced in the same way, with approximately half of them arranged below and above region B. The regions A_i need not have the same widths. The power functions, ϑ^{k-1}, shall be chosen to some extent as above as the functions $\psi_k(\vartheta)$. For the same purpose, the functional shapes of the disturbing neighbouring lines that have to be considered should also be chosen as far as possible and known. One shall proceed according to C.1 and $\tilde{u}^2(\tilde{y})$ again follows from Equation (C.5).

After the calculation of $\tilde{u}^2(\tilde{y})$ in all cases according to Equation (C.5), the characteristic limits result with Equation (C.4) and according to Clause 6.



Key

ϑ energy, time, etc.

v counted content of each of the channels

For the curves, see the text.

Figure C.1 — Arrangement of the channel regions for the determination of the background of a line

Figure C.1 shows the arrangement scheme of the adjacent channel regions, $A_i\,(i = 1, 2, 3, 4)$, in the multi-channel spectrum for the determination of a weakly curved background of a line in region B [case c)]. The regions A_i have the contents, n_i, and the same width, t, region B has the content, n_g, and the width, $t_g = 2{,}5h$, with the full width, h, at half-maximum. The abscissa, ϑ, for instance, energy or time, is assigned to the channel number and $\bar{\vartheta}_g$ is its value in the middle of region B. The ordinate, v, denotes the counted content of each of the channels. With a constant or linear background, only two regions A'_i arranged in the order A'_1, B, A'_2 are needed [cases a) and b)]. The straight line b and the cubic parabola c represent the background shape of the line in the spectrum. They are determined according to C.3 for cases b) and c), respectively. For case b), regions A_1 and A_2 have been combined to form A'_1 with the width, $2t$, and, likewise, regions A_3 and A_4 to form A'_2. The straight line b does not fulfil the chi-square condition (see D.5). Lines d: unfolded spectrum of the regions A_i and B and related background according to C.5 (see also D.5.3). In the example shown, the background lines b and d nearly coincide in region B.

C.3 Obtaining the regions for determining the background

The regions A_i for background determination can be obtained by performing a test on whether or not the function $H(\vartheta)$ can represent the background shape. For this purpose and with the total number, $M > m$, of all channels of regions A_i, with the counted content, v_j, of channel $v_j\,(j = 1, ..., M)$ of these regions, with the value $\bar{\vartheta}_j$ of the scaling variable, ϑ, assigned to the middle of the channel, j, and with the channel width, $\Delta\vartheta_j$, the test quantity

$$\chi^2 = \sum_{j=1}^{M} \frac{\left[H(\bar{\vartheta}_j; a_1, ..., a_m)\Delta\vartheta_j - v_j \right]^2}{v_j + 1} \tag{C.13}$$

is calculated. Then it is ascertained whether or not

$$\left| \chi^2 - M + m \right| \leqslant k_{1-\delta/2}\sqrt{2(M-m)} \tag{C.14}$$

The error probability, $\delta = 0{,}05$, is recommended. Depending on whether the chi-square condition according to Equation (C.14) for the compatibility of the function $H(\vartheta)$ with the measured background shape in the regions A_i of the spectrum is fulfilled or not, the regions A_i and thus M shall be enlarged or reduced, respectively, and the test shall be repeated until maximum regions still compatible with the condition are found.

If functional values, $H(\vartheta)$, are negative in the regions A_i and B, the procedure is not applicable in the way described here. For the denominator $v_j + 1$ in Equation (C.13), see under Equation (F.1).

In cases a) to c), the function $H(\vartheta)$ can be explicitly specified:

case a) $$H(\vartheta) = \frac{n_0}{t_0} \tag{C.15}$$

case b) $$H(\vartheta) = \frac{n_0}{t_0} + \frac{4(n_2 - n_1)(\vartheta - \bar{\vartheta}_g)}{t_0(2t_g + t_0)} \tag{C.16}$$

case c) $$H(\vartheta) = a_1 + a_2(\vartheta - \bar{\vartheta}_g) + a_3(\vartheta - \bar{\vartheta}_g)^2 + a_4(\vartheta - \bar{\vartheta}_g)^3 \tag{C.17}$$

where $\bar{\vartheta}_g$ is the value of ϑ assigned to the middle of region B and, moreover,

$$\begin{aligned} a_1 &= \frac{n_0}{t_0} - \frac{4n_0'(t_g^2 + t_g t_0 + t_0^2/3)}{t_0^2(2t_g + t_0)} \;;\quad a_2 = 16\frac{n_3 - n_2}{t_0(4t_g + t_0)} - \frac{a_4}{32}\left[(2t_g + t_0)^2 + (2t_g)^2 \right] ; \\ a_3 &= \frac{16n_0'}{t_0^2(2t_g + t_0)} \;;\quad a_4 = 256\frac{(n_4 - n_1)(4t_g + t_0) - (n_3 - n_2)(4t_g + 3t_0)}{t_0^2(4t_g + t_0)(4t_g + 2t_0)(4t_g + 3t_0)} \end{aligned} \tag{C.18}$$

As a numerical example, Figure C.1 shows a section of a multi-channel spectrum, recorded using a NaI detector, with the background shapes calculated according to cases b) and c). For more details, see D.5.2.

C.4 Extending applications

From the net line intensity obtained according to Equations (C.1) and (C.2) and in combination or comparison with further quantities (for instance calibration, correction or influence quantities or conversion factors such as sample mass, emission or response probability), another measurand of interest often has to be calculated.

This can be, for instance, an activity (concentration) or the quotient of the net line intensity and the net intensity of a reference line in the same spectrum or the net intensity of the same line in a reference spectrum. In such cases, after the calculations according to Equations (C.1) and (C.2) have been carried out, proceed in essence according to 5.2 and 5.3 as follows.

In 5.2 and 5.3, the measurand, Y, of interest and the input quantities, X_i, appear. They shall be specified according to the following equations, where on the left-hand side one of the aforementioned quantities and on the right-hand side the respective quantity according to Equation (C.1) are found.

If Y is an activity (concentration) or an analogous quantity, $X_1 = X_g$ and $X_2 = Z_0$ and $X_3 = 1$ are set. Moreover, $x_5 = 1$ or 0,84 and $u(x_5) = 0$, if Equations (C.9) and (C.10), respectively, are used. Further input quantities, X_i, are specified as conversion factors.

If $Y = Y_1/Y_2$ is the quotient of the net line intensity Y_1, determined according to Equations (C.1) and (C.2), and the likewise determined net intensity, Y_2, of a reference line in the same or a different spectrum, $X_1 = Y_1$ and $X_2 = 0$ and $X_5 = Y_2$ are specified.

To correct a spectrometric superposition of the line of interest by a disturbing line, L, with the same energy, but from a different nuclide, one shall proceed in a way similar to the preceding paragraph. Then $X_1 = Y_1$ is the net intensity sum of both lines and $X_2 = Y_2$ is the net intensity of a line of the disturbing nuclide that serves as a reference. With the presumption that the spectrum of this nuclide can be separately measured free from the line of interest, for instance, on a blank, two cases shall be distinguished. In the first case, the disturbing line, L, itself serves as a reference. Then $x_3 = t_1/t_2$ and $u(x_3) = 0$ for X_3 shall be specified, where t_1 and t_2 are the measurement durations of the spectra. In the second case, another line, L', of the disturbing nuclide in the spectrum to be examined serves as a reference. Then the net intensities, i and i', of the lines, L and L', respectively, and the associated standard uncertainties, $u(i)$ and $u(i')$, shall be determined from the separately measured spectrum, and the following shall be specified:

$$x_3 = \frac{i}{i'} \; ; \quad u^2(x_3) = x_3^2 \cdot \left[\frac{u^2(i)}{i^2} + \frac{u^2(i')}{i'^2} \right] \tag{C.19}$$

C.5 Unfolding in spectrometric measurements

C.5.1 Special quantities and symbols used in this Clause

i channel number of a channel in a multi-channel spectrum obtained by a spectrometric nuclear radiation measurement $(i = 1, ..., m)$

ϑ continuous parameter (for example energy or time) related to the different channels in a multi-channel spectrum

ϑ_i value of ϑ connected with channel i $(i = 1, ..., m)$

t duration of measurement

m number of channels in the spectrum

N_i Poisson-distributed random variable of events counted in channel, i, during the measuring time, t $(i = 1, ..., m)$

n_i number of events counted in a channel, i, during the measuring time, t $(i = 1, ..., m)$, estimate of N_i

X_i random variable of the rate of events counted in channel i during the measuring time, t, input quantity of the evaluation, $X_i = N_i/t \quad (i = 1, ..., m)$

$\boldsymbol{X}$ column matrix of the X_i

x_i rate of events counted in channel, i, during the measuring time, t, $x_i = n_i/t \quad (i = 1, ..., m)$, estimate of X_i

$\boldsymbol{x}$ column matrix of the x_i

$u(x_i, x_j)$ covariance associated with x_i and x_j

Y_k output quantity (parameter) derived from the multi-channel spectrum by unfolding methods $(k = 1, ..., n)$

$\boldsymbol{Y}$ column matrix of the Y_k

y_k estimate of the output quantity $Y_k \quad (k = 1, ..., n)$

$u(y_k)$ standard uncertainty associated with y_k

$\tilde{\boldsymbol{y}}$ column matrix $\boldsymbol{y}$ after replacement of y_1 with $\tilde{y}$

$\boldsymbol{z}$ column matrix of values z_i fitted to the values x_i

$H(\vartheta_i)$ functional relationship representing the spectral density at ϑ_i of a multi-channel spectrum

$\psi_k(\vartheta)$ function describing the shape of an individual spectral line or of a background contribution $(k = 1, ..., n)$

n number of output quantities

p_i estimate of an input quantity which is not subject to fit

$\boldsymbol{p}$ column matrix of the p_i

$\boldsymbol{w}$ column matrix of input estimates; $\boldsymbol{w} = (x_1, ..., x_m, p_1, p_2, ...)^{\mathrm{T}}$ (transposed row matrix)

$\boldsymbol{A}$ response matrix of the spectrometer

A_{ik} elements of the response matrix $\boldsymbol{A}$

$\boldsymbol{U}_{\boldsymbol{x}}$ uncertainty matrix of $\boldsymbol{X}$

$\boldsymbol{U}_{y}$ uncertainty matrix of $\boldsymbol{Y}$

G_k function of the input quantities $X_i \quad (i = 1, ..., m)$

$\boldsymbol{G}$ column matrix of the G_k

diag indicator for a diagonal matrix

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C.5.2 Model of unfolding and general uncertainty treatment

For the unfolding of spectrometric measurements, the model of the evaluation shall be written more general than in 5.2.1, allowing for more than a single measurand and for correlated quantities. In this case, the model is given by a set of n functional relationships:

$$Y_k = G_k(X_1, ..., X_m); \quad (k = 1, ..., n) \tag{C.20}$$

Estimates y_k of the n measurands Y_k are obtained from Equation (C.20) by inserting estimates x_i for the m input quantities X_i ($i = 1, ..., m$):

$$y_k = G_k(x_1, ..., x_m); \quad (k = 1, ..., n) \tag{C.21}$$

The standard uncertainties, $u(x_i)$, and covariances, $u(x_i,x_j)$, associated with the x_i are the elements of the symmetric uncertainty matrix $\boldsymbol{U}_{\boldsymbol{x}}$ and meet the relations $u(x_i,x_i) = u^2(x_i)$ and $u(x_i,x_j) = u(x_j,x_i)$. If they are given, the analogous standard uncertainties $u(y_k)$ and covariances $u(y_k,y_l)$ associated with the y_k follow from:

$$u(y_k,y_l) = \sum_{i,j=1}^{m} \frac{\partial G_k}{\partial x_i} \cdot \frac{\partial G_l}{\partial x_j} \cdot u(x_i,x_j); \quad (k,l = 1, ..., n) \tag{C.22}$$

One obtains $u(y_k) = \sqrt{u(y_k,y_k)}$ and $u(y_k,y_l) = u(y_l,y_k)$ ($k \neq l$). For convenience, the partial derivatives $\partial G_k / \partial X_i$ with all the input quantities X_i substituted by their estimates x_i are briefly denoted by $\partial G_k / \partial x_i$ in Equation (C.22) and in the following.

The model functions G_k need not be explicitly available as arithmetical expressions. They can also be given as an algorithm, for instance, in form of a computer code. In such cases, or when more complicated model functions are involved, the partial derivatives possibly cannot be explicitly derived but can numerically be approximated sufficiently exactly using half of the standard uncertainty $u(x_i)$ as an increment of x_i:

$$\frac{\partial G_k}{\partial x_i} = \frac{1}{u(x_i)} \left\{ G_k\left[x_1, ..., x_i + u(x_i)/2, ..., x_m\right] - G_k\left[x_1, ..., x_i - u(x_i)/2, ..., x_m\right] \right\} \tag{C.23}$$

NOTE Equations (C.21) to (C.23) apply for model functions G_k which can be taken as sufficiently linear in the uncertainty ranges between $x_i - u(x_i)$ and $x_i + u(x_i)$. Otherwise, more refined procedures can be applied as described in ISO/IEC Guide 98-3:2008, 5.1.2 Note (see also References [1, Annex C]; [2, Annex E]; [6]; [7]; 16]).

In spectrum unfolding, it is convenient to use matrix notation. Therefore, those quantities, values and functions being denoted by the same symbol are in the following combined to form a column matrix, written as a transposed row matrix and denoted by the same symbol, but in bold face. Examples are $\boldsymbol{x} = (x_1, ..., x_m)^{\mathsf{T}}$ and $\boldsymbol{y} = (y_1, ..., y_n)^{\mathsf{T}}$ and $\boldsymbol{G}(\boldsymbol{x}) = (G_1, ..., G_n)^{\mathsf{T}}$. In addition, the uncertainty matrices $\boldsymbol{U}_x = [u(x_i,x_j)]$ and $\boldsymbol{U}_y = [u(y_k,y_l)]$ and also the sensitivity matrix $\boldsymbol{G}_{\boldsymbol{x}} = (\partial G_k / \partial x_i)$ are introduced. Equations (C.21) and (C.22) then quickly read:

$$\boldsymbol{y} = \boldsymbol{G}(\boldsymbol{x}); \quad \boldsymbol{U}_{\boldsymbol{y}} = \boldsymbol{G}_{\boldsymbol{x}} \boldsymbol{U}_{\boldsymbol{x}} \boldsymbol{G}_{\boldsymbol{x}}^{\mathsf{T}} \tag{C.24}$$

C.5.3 Spectrum unfolding in nuclear spectrometric measurement

The evaluation of a nuclear spectrometric measurement usually is an (in general, non-linear) unfolding of a measured multi-channel spectrum. It can also comprise the unfolding of several measured spectra and consideration of other data. Such an evaluation is commonly called spectrum unfolding.

The input quantities, X_i, of the spectrum unfolding are all quantities from which measured data or other data are used in the unfolding and which have uncertainties associated with them. These are all those quantities, X_i, for which a measured or estimated value, x_i, is available and which shall be fitted in the unfolding procedure. One of those quantities, X_i, is to be assigned to each individual channel, i, of a multi-channel spectrum, where n_i events are counted during a measuring time, t. Likewise, an input quantity, X_i, shall be assigned to each

parameter to be determined for which an estimate is given before the evaluation. Examples are spectrum parameters such as the widths of spectral lines or parameters of the sensitivity matrix of the spectrometer.

For a count rate $X_i = \rho_i$ with the given counting result, n_i, recorded during the measuring time, t, and if independent Poisson statistics can be assumed for the individual channels, the specifications $x_i = r_i = n_i/t$ and $u^2(x_i) = n_i/t^2 = x_i/t$ apply as in 5.2.1 (see F.1, in particular, if $n_i = 0$). In addition, the covariances can be set at zero, i.e. $u(x_i,x_j) = 0$ $(i \neq j)$. It is possible for the measuring times associated with the individual channels to not necessarily be identical. The components of uncertainty of measurement comprise uncertainty matrices $\boldsymbol{U_x} = [u(x_i,x_j)]$ and $\boldsymbol{U_y} = [u(y_k,y_l)]$. $\boldsymbol{U_x}$ is diagonal with the diagonal elements $u^2(x_i) = n_i / t^2$, i.e. $\boldsymbol{U_x} = \mathrm{diag}(x_i / t)$.

Further, there are input quantities for which estimates p_i are available, but which are not subject to fit. These include, for instance, base points, calibration parameters, correction and influence quantities or other parameters which were already previously mentioned. The values ϑ_i connected with channel i of the parameter ϑ related to the different channels in a multi-channel spectrum are such quantities.

In principle, all quantities for which an estimate is given should be fitted. Frequently, however, this is not technically feasible or some quantities were determined from other experiments, such that it is not meaningful to fit them too. Such quantities which are known sufficiently exactly so that their uncertainties are negligible are not treated as input quantities but as constants. If only the Poisson statistics of the channel counts of a multi-channel spectrum should be considered, only these quantities are input quantities. In this case, all other quantities are constants.

The output quantities, Y_k, of the spectrum unfolding are the parameters of the unfolding which shall be determined. The measurand, for which decision threshold, detection limit and the limits of a confidence interval shall be determined, is one of them. The number of these parameters should be as small as possible. The output quantities can also be spectrum parameters such as net areas of spectral lines or the number of background counts under a spectral line or in a particular channel or unknown parameters of the sensitivity matrix.

For convenience, the estimates $\boldsymbol{x}$ and $\boldsymbol{p}$ are combined to form the column matrix $\boldsymbol{w} = (x_1, ..., x_m, p_1, p_2, ...)^T$.

For the unfolding, one needs the estimates, $\boldsymbol{x}$ and $\boldsymbol{p}$, of the input quantities and their associated uncertainty matrix, $\boldsymbol{U_w}(\boldsymbol{x},\boldsymbol{p})$. This uncertainty matrix has been calculated as a covariance matrix based on ISO/IEC Guide 98-3 (see References [1, 2]). The uncertainty matrix, $\boldsymbol{U_w}(\boldsymbol{x},\boldsymbol{p})$, is needed in form of its functional dependence on $\boldsymbol{x}$ since $\boldsymbol{x}$ shall be adjusted if decision threshold and detection limit are calculated while $\boldsymbol{p}$ stays constant. The uncertainty matrices $\boldsymbol{U_x}$ and $\boldsymbol{U_p}$ associated with $\boldsymbol{x}$ and $\boldsymbol{p}$ are partial matrices of $\boldsymbol{U_w}$. The rank of $\boldsymbol{U_x}$ shall not be smaller than the number n of model equations. If the data for $\boldsymbol{x}$ and $\boldsymbol{p}$ originate from different independent experiments, there is no correlation between $\boldsymbol{x}$ and $\boldsymbol{p}$ and the matrix elements of $\boldsymbol{U_w}$ related to pairs x_i and p_k vanish.

A more detailed description of spectrum unfolding in nuclear spectrometric measurements is given in References [17, 31, 32].

The model of the unfolding consists of n relationships between input and output quantities. These relationships can formally and most generally be written as a column matrix $\boldsymbol{H}(\boldsymbol{y},\boldsymbol{p})$ of model functions H_k which depend on all these quantities.

$$\boldsymbol{x} = \boldsymbol{H}(\boldsymbol{y},\boldsymbol{p}) \tag{C.25}$$

If an output quantity, Y_i, is likewise an input quantity, X_i, for which an estimate, x_i, is given, the equation $x_i = y_i$ shall be added to the model functions. If output quantities, such as activity, particle fluence or equivalent dose, depend on other output quantities, the respective functional dependencies shall also be added to the model functions. The model functions shall not be explicitly available as mathematical expressions. They can also be an algorithm, for instance in form of a computer code of the evaluation.

For the unfolding of a measured multi-channel spectrum, one fits functions $\boldsymbol{H}(\boldsymbol{Y})$ according to Equation (C.25) to the estimates $\boldsymbol{x}$ of the m input quantities $\boldsymbol{X}$; for instance to the measured values $x_i = n_i / t$ of the spectral density calculated from the channel counts n_i.

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The calculation of the estimates $\boldsymbol{y}$ of the output quantities, $\boldsymbol{Y}$, of the uncertainty matrix, $\boldsymbol{U_y}$, associated with $\boldsymbol{y}$ and of the fitted values $\boldsymbol{z}$ (best estimate), of the input quantities, $\boldsymbol{X}$, from the given measured and estimated values of all input quantities, $\boldsymbol{w}$, with their associated uncertainty matrix, $\boldsymbol{U_w}$, is in general a non-linear fitting procedure the solution of which is described in C.5.4.

In the special case of a spectrum unfolding which is linear in the parameters $\boldsymbol{Y}$, the spectral density $H(\vartheta_i)$ is represented by the column matrix $\boldsymbol{X} = [H(\vartheta_i)]$. The ϑ_i are assumingly exact base points, for instance the energies or times assigned to the individual channels. The spectral density is approximated by a system of functions $\psi_k(\vartheta)$:

$$X_i = H(\vartheta_i) = \sum_{k=1}^{n} \psi_k(\vartheta_i) \cdot Y_k \; ; (i = 1, ..., m) \quad \text{or} \quad \boldsymbol{X} = \boldsymbol{A}\boldsymbol{Y} \tag{C.26}$$

The constant response matrix $\boldsymbol{A}$ consists of the elements $A_{ik} = \psi_k(\vartheta_i)$. The functions $\psi_k(\vartheta_i)$ describe the shapes of the individual spectral lines and of the background contributions. (For explicit examples of $\psi_k(\vartheta_i)$ when evaluating alpha- and gamma-spectra, see C.5.5 and C.5.6.) The output quantities, Y_k, to be determined are for instance the net peak areas of the spectral lines.

C.5.4 Procedure for spectrum unfolding

A spectrum unfolding means in essence fitting new values, $\boldsymbol{z}$, of the input quantities, $\boldsymbol{X}$, to the given estimates, $\boldsymbol{x}$ where $\boldsymbol{z} = \boldsymbol{H}(\boldsymbol{y},\boldsymbol{p})$ depends on the measurand estimates, $\boldsymbol{y}$, to be determined and on fixed given estimates, $\boldsymbol{p}$, of further input quantities which are not subject to fit. The generalized least-squares method is highly recommended for use as a spectrum unfolding procedure since it can easily be combined with the uncertainty treatment and allows for a compact and transparent description as follows.

The measurand estimates, $\boldsymbol{y}$, are determined by minimizing the quantity

$$\chi^2 = (\boldsymbol{x} - \boldsymbol{z})^{\mathsf{T}} \boldsymbol{U}_{\boldsymbol{x}}^{-1}(\boldsymbol{x})(\boldsymbol{x} - \boldsymbol{z}) = \min \tag{C.27}$$

with the constraint $\boldsymbol{z} = \boldsymbol{H}(\boldsymbol{y},\boldsymbol{p})$ and the uncertainty matrix, $\boldsymbol{U}_x(\boldsymbol{x})$, given as a function of $\boldsymbol{x}$ for finally obtaining the characteristic limits. The results of this minimizing procedure are the functions:

$$\boldsymbol{y} = \boldsymbol{G}(\boldsymbol{x}, \boldsymbol{p}) = \boldsymbol{G}(\boldsymbol{w}) \tag{C.28}$$

$$\boldsymbol{z} = \boldsymbol{H}(\boldsymbol{y}, \boldsymbol{p}) = \boldsymbol{H}\left[\boldsymbol{G}(\boldsymbol{w}), \boldsymbol{p}\right] = \boldsymbol{F}(\boldsymbol{w}) \tag{C.29}$$

and, similar to Equation (C.24) where $\boldsymbol{w}$ now plays the part of $\boldsymbol{x}$, the due uncertainty matrices:

$$\boldsymbol{U}_y = \boldsymbol{G}_{\boldsymbol{w}} \boldsymbol{U}_{\boldsymbol{w}} \boldsymbol{G}_{\boldsymbol{w}}^{\mathsf{T}} \; ; \quad \boldsymbol{U}_z = \boldsymbol{F}_{\boldsymbol{w}} \boldsymbol{U}_{\boldsymbol{w}} \boldsymbol{F}_{\boldsymbol{w}}^{\mathsf{T}} \tag{C.30}$$

Here, $\boldsymbol{x}$ and $\boldsymbol{p}$ are combined to form the column matrix, $\boldsymbol{w}$. The uncertainty matrices, $\boldsymbol{U}_{\boldsymbol{x}}$ and $\boldsymbol{U}_{\boldsymbol{p}}$, are likewise combined to form the uncertainty matrix, $\boldsymbol{U}_{\boldsymbol{w}}$. The sensitivity matrices, $\boldsymbol{F}_{\boldsymbol{w}}$ and $\boldsymbol{G}_{\boldsymbol{w}}$, denote the matrices of the partial derivatives of the functions $\boldsymbol{F}(\boldsymbol{w})$ and $\boldsymbol{G}(\boldsymbol{w})$, respectively. All the matrices on the right-hand side of Equation (C.30) are functions of $\boldsymbol{w}$.

The results of the fit and the given data $\boldsymbol{x}$ conform if the standardized chi-square χ_s^2 meets, with $m > n$ and with the obtained minimum $\chi_{\min}^2$, the chi-square condition:

$$\chi_s^2 = \frac{\left|\chi_{\min}^2 - (m-n)\right|}{\sqrt{2(m-n)}} \leqslant k_{1-\delta/2} \tag{C.31}$$

The error probability $\delta = 0{,}05$ is recommended.

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The standard uncertainty function, $\tilde{u}(\tilde{y})$, of the true value, $\tilde{y}$, of the measurand, Y, in question for which the characteristic limits are to be determined, say, $Y = Y_1$, can be obtained in the following way. The estimate, y_1, is first replaced with $\tilde{y}$ yielding $\tilde{\boldsymbol{y}} = (\tilde{y}, y_2, ..., y_n)^{\mathsf{T}}$, which is now used instead of $\boldsymbol{y}$. This leads to $\tilde{\boldsymbol{z}} = \boldsymbol{H}(\tilde{\boldsymbol{y}}, \boldsymbol{p})$, replacing the column matrix $\boldsymbol{x}$. Thus, the column matrix $\tilde{\boldsymbol{w}}$ follows as the combination of $\tilde{\boldsymbol{z}}$ and $\boldsymbol{p}$ and, moreover, $\tilde{\boldsymbol{U}}_{\boldsymbol{w}}$ follows as the combination of $\boldsymbol{U}_{\boldsymbol{x}}(\tilde{\boldsymbol{z}})$ and $\boldsymbol{U}_{\boldsymbol{p}}$. The matrices $\tilde{\boldsymbol{w}}$ and $\tilde{\boldsymbol{U}}_{\boldsymbol{w}}$ are used in Equation (C.30) instead of $\boldsymbol{w}$ and $\boldsymbol{U}_{\boldsymbol{w}}$ to calculate $\tilde{\boldsymbol{U}}_{\boldsymbol{y}}$. Finally, the square root of the (1,1)-element of this uncertainty matrix is the needed function $\tilde{u}(\tilde{y})$.

In many cases, the function $\boldsymbol{H}(\boldsymbol{y},\boldsymbol{p})$ to be adapted to the given estimates $\boldsymbol{x}$ is linear in $\boldsymbol{y}$, i.e., $\boldsymbol{z} = \boldsymbol{H}(\boldsymbol{y},\boldsymbol{p}) = \boldsymbol{A}\boldsymbol{y}$ where the matrix $\boldsymbol{A}$ does not depend on $\boldsymbol{p}$ and can represent the spectrometer response. Then $\boldsymbol{x}$ and $\boldsymbol{w}$ are identical and the minimizing procedure of the least-squares method can easily be carried out and results in

$$\boldsymbol{y} = \boldsymbol{U}_{\boldsymbol{y}}\boldsymbol{A}^{\mathsf{T}}\boldsymbol{U}_{\boldsymbol{x}}^{-1}(\boldsymbol{x})\boldsymbol{x}\,; \quad \boldsymbol{U}_{\boldsymbol{y}} = \left[\boldsymbol{A}^{\mathsf{T}}\boldsymbol{U}_{\boldsymbol{x}}^{-1}(\boldsymbol{x})\boldsymbol{A}\right]^{-1} \tag{C.32}$$

$$\boldsymbol{z} = \boldsymbol{A}\boldsymbol{y}\,; \quad \boldsymbol{U}_{\boldsymbol{z}} = \boldsymbol{A}\boldsymbol{U}_{\boldsymbol{y}}\boldsymbol{A}^{\mathsf{T}} \tag{C.33}$$

$$\chi^2_{\min} = \boldsymbol{x}^{\mathsf{T}}\boldsymbol{U}_{\boldsymbol{x}}^{-1}(\boldsymbol{x})(\boldsymbol{x}-\boldsymbol{z})\,; \quad \tilde{\boldsymbol{U}}_{\boldsymbol{y}} = \left[\boldsymbol{A}^{\mathsf{T}}\boldsymbol{U}_{\boldsymbol{x}}^{-1}(\boldsymbol{A}\tilde{\boldsymbol{y}})\boldsymbol{A}\right]^{-1} \tag{C.34}$$

C.5.5 Application to alpha-spectrometry

In many cases of alpha-spectrometry, an alpha-spectrum measured by a semiconductor detector or a grid ionisation chamber can be considered to be a superposition of individual spectral lines, usually without a background contribution. In this case, a linear model of the type $\boldsymbol{x} = \boldsymbol{A}(\boldsymbol{p})\boldsymbol{y}$ can be used. The following functional representation can be used for the shape of a spectral line j (see References [33-37]):

$$L_j(E) = \int_{-\infty}^{\infty} \frac{R_j(E')}{\sqrt{2\pi\sigma_j^2}} \exp\left[-\frac{(E'-E)^2}{2\sigma_j^2}\right] \mathrm{d}E'$$

$$R_j(E) = \alpha_{0,j} \cdot \delta(E - E_{0,j}) + \sum_{k=1}^{3} (\alpha_{k,j}/\tau_{k,j}) \cdot \exp\left[(E - E_{0,j})/\tau_{k,j}\right] \quad \text{for } (E \leqslant E_{0,j}) \tag{C.35}$$

$$R_j(E) = 0 \quad \text{for } (E > E_{0,j})$$

$$\alpha_{0,j} + \alpha_{1,j} + \alpha_{2,j} + \alpha_{3,j} = 1$$

E is the energy of the alpha-particles. All other quantities are given parameters of the spectral line. These parameters of all spectral lines, as well as the parameters of the energy calibration which connects the channel number i and the energy E are input quantity estimates, $\boldsymbol{p}$, or are considered to be known constants. The elements of the response matrix are $A_{ij} = L_j(E_i)$, with E_i being the energy associated with channel i.

The spectral line at alpha-energy $E_{0,j}$ is physically characterized by the first term of $R_j(E)$, the delta function, in Equation (C.35). The three following terms describe the energy loss of the alpha-particles on their path to detection. The folding integral in the first line of Equation (C.35) considers the resolution, σ, of the spectrometer which usually depends on E.

The parameters y_j to be determined are the peak areas. They form the column matrix $\boldsymbol{y}$ of the output quantities. One of them is the quantity Y in question. For the spectrum one hence receives the functional expression $x_i = \sum_j L_j(E_i) \cdot y_i$ or, written as a matrix, $\boldsymbol{x} = \boldsymbol{A}(\boldsymbol{p})\boldsymbol{y}$.

If some of the parameters $\boldsymbol{p}$, for instance the location of the spectral lines or parameters of the peak shape, are not known, but are likewise to be determined by the unfolding, these unknown quantities are to be added to the output quantities $\boldsymbol{y}$. Then, $\boldsymbol{A}$ depends also on $\boldsymbol{y}$ and one obtains the case of a non-linear model according to Equation (C.25) with $\boldsymbol{x} = \boldsymbol{H}(\boldsymbol{y},\boldsymbol{p}) = \boldsymbol{A}(\boldsymbol{y},\boldsymbol{p})\boldsymbol{y}$.

The functions $L_j(E)$ are the response functions of the spectrometer which can, for instance, be a semiconductor detector or a grid ionisation chamber in alpha-spectrometry, but also a semiconductor detector in gamma-spectrometry or a Bonner sphere in neutron spectrometry. Mathematically, they can be nearly arbitrarily chosen and therefore they can be set up as required for phenomenological or physical reasons. They can also be measured functions or calculated ones which reflect the underlying physical processes. They can be known as analytical expressions as well as numerical. With these response functions, it is not only possible to describe shapes of spectral lines. Also, the background under spectral lines can be modelled by superposition of such functions in any arbitrary way. For its application to gamma-spectrometric measurements, see C.5.6.

C.5.6 Application to gamma-spectrometry

In gamma-spectrometry, background contributions generally shall not be neglected. In spite of that a linear model of the type $\boldsymbol{x} = \boldsymbol{A}(\boldsymbol{p})\boldsymbol{y}$ can be set up using the general procedure in C.1. The following functional representation can be used to describe the superposition of contributions from spectral lines and background in a part of the spectrum under investigation:

$$L_1(E) = \exp\left[-(E - E_0)^2/(2\sigma^2)\right]/\sqrt{2\pi\sigma^2}$$

$$L_2(E) = \arctan\left[-(E - E_0)/a\right] \qquad \text{(C.36)}$$

$$L_j(E) = (E - E_0)^{j-3}\ ; \quad (j = 3,4,5,6)$$

The first function in Equation (C.36) describes the shape of a spectral line by a Gaussian function with a spectrometer resolution, σ. In actual cases, more complicated line shapes may be used, introducing, for instance, low-energy exponential tailings, which increases the number of parameters of the peak shape. The second line of Equation (C.36) represents a "step function" under a spectral line which shall be explained as a consequence of incomplete charge collection. a is a parameter characterizing the steepness of the step function and shall be known beforehand. The residual functions in the third line of Equation (C.36) are used to model phenomenologically the background by a third order polynomial. Instead of the energy E, the channel number i can also be used in the set-up of the model according to Equation (C.36).

E is the energy deposited in the detector. All other quantities are parameters of the spectral line or of the background step function. These parameters, σ and a, of all spectral lines, as well as of the energy calibration which connects the channel number i and the energy E, are input quantities $\boldsymbol{p}$ or are considered to be known constants. The elements of the response matrix are $A_{ij} = L_j(E_i)$, with E_i being the energy associated with channel i.

The parameters y_j to be determined are the peak areas and the background contributions. They form the column matrix $\boldsymbol{y}$ of the measurand estimates. One of the peak areas is the quantity Y in question. For the spectrum, one hence receives the functional expression $x_i = \sum_j L_j(E_i) \cdot y_i$ or, in matrix notation, $\boldsymbol{x} = \boldsymbol{A}(\boldsymbol{p})\boldsymbol{y}$.

In contrast to alpha-spectrometry, in gamma-spectrometry frequently some of the parameters $\boldsymbol{p}$ are not known exactly, for instance, the location of the spectral lines or parameters of the peak or background shape. Starting from estimates, they are likewise to be determined by the unfolding. Consequently, these unknown quantities are to be added to the output quantities, $\boldsymbol{y}$. Then, $\boldsymbol{A}$ depends also on $\boldsymbol{y}$ and one obtains the case, which is usual in complex gamma-spectrometry, of a non-linear model according to Equation (C.25) with $\boldsymbol{x} = \boldsymbol{H}(\boldsymbol{y},\boldsymbol{p}) = \boldsymbol{A}(\boldsymbol{y},\boldsymbol{p})\boldsymbol{y}$.

A numerical example of unfolding a gamma spectrum is discussed in D.5.3.

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Annex D
(informative)

Application examples

D.1 General aspects

This annex gives numerical examples of the applications discussed in Annexes B and C. The respective equations used for the calculations are referred to. In all examples, y, $u(y)$ and $\tilde{u}(\tilde{y})$ are first determined and then the characteristic limits, as well as the best estimate of the measurand with the associated standard uncertainty, are calculated according to the equations given in Clause 6 or A.5 to A.8 and by applying Annex E.

The data in Tables D.1 to D.4 are often given with more digits than are meaningful, so that the calculations can also be reconsidered and verified with higher accuracy, in particular for testing computer programs under development. Some intermediate values, which shall be calculated in a more complicated way, are also given for test purposes.

The examples are not intended to standardize measurement procedures in the respective applications and can only serve as explanations for the application of this International Standard.

D.2 Example 1: Measurement of an alpha-activity concentration

D.2.1 Counting measurement

This generic example deals with the examination of an alpha-activity in a liquid material by means of a direct deposition on a planchet and a subsequent counting measurement of the alpha-particles. The measurand, Y, is the alpha-activity concentration c_A (activity divided by volume). For this task, the characteristic limits, the best estimate and the associated standard uncertainty shall be calculated. The model of the evaluation in this case reads according to Equation (4):

$$Y = c_A = \frac{X_1 - X_2}{X_5 X_7 X_9} = \frac{r_g - r_0}{V \cdot \varepsilon \cdot f} \tag{D.1}$$

$X_1 = r_g$ is the gross count rate and $X_2 = r_0$ is the background count rate; $X_5 = V$ is the volume from which the activity has been deposited on the planchet; $X_7 = \varepsilon$ is the detection efficiency and $X_9 = f$ is the self-absorption factor of the alpha-particles in the deposited material.

After the counting measurements of the gross effect and of the background effect are carried out with the respective measurement durations t_g and t_0, the respective numbers n_g and n_0 of the recorded events are available. These numbers are used according to 5.2.2 to specify the estimate $x_1 = r_g = n_g/t_g$ with $u^2(x_1) = n_g/t_g^2 = r_g/t_g$ for the gross count rate X_1 and $x_2 = r_0 = n_0/t_0$ with $u^2(x_2) = n_0/t_0^2 = r_0/t_0$ for the background count rate X_2. These specifications apply to measurements with time preselection.

The detection efficiency, $\varepsilon = 0{,}3$, is determined using a calibration source with a certified relative standard uncertainty of 5 %. On the assumption that the statistical contribution to the measurement uncertainty of the detection efficiency is negligible, $u(\varepsilon) = 0{,}015$ results.

It is known from previous experiments that the self-absorption factor, f, of the alpha-particles in different, not further specified deposited materials is randomly distributed between 0,4 and 0,8. This yields the mean estimate $f = 0{,}6$ and the associated standard uncertainty, $u(f) = \Delta f / \sqrt{12}$, by specifying a rectangular

distribution over the region of the possible values of f with the width $\Delta f = 0{,}40$ (see 5.2.2, second-to-last paragraph). The self-absorption factor, f, has a rather large relative standard uncertainty, $u(f)/f = 0{,}19$, and the measurand depends reciprocally on it. Therefore, an influence of non-linearity should be expected (see C.5.2 Note).

The relative standard uncertainty of the sampled volume, $V = 0{,}5$ l, is given as 1 % from experience, leading to $u(V) = 0{,}005$ l.

For the input data, specifications, some intermediate values and results, see Table D.1. The results are calculated according to 5.2.2, 5.3.2 and Clause 6. In particular, Equations (6), (9) and (14) are used for y, $u(y)$ and $\tilde{u}(\tilde{y})$, respectively, where $x_3 = 1$, $u(x_3) = 0$, $x_4 = 0$ and $u(x_4) = 0$ are set because X_3 and X_4 are not involved in the model. Some standard uncertainties are not given in Table D.1 since they are not explicitly needed for the equations.

D.2.2 Measurement using a ratemeter

The measurement of the count rate can also be carried out using a ratemeter (see B.3). In contrast to D.2.1, $u^2(x_1) = r_g/(2\tau_g)$ and $u^2(x_2) = r_0/(2\tau_0)$ here apply. For an easy comparison in Table D.1, the input data of the ratemeter measurement are fictitiously chosen such that the primary measurement result, y, is almost unchanged when compared with that of the counting measurement. The relaxation time constants strongly influence the decision threshold and the detection limit. Their values $\tau_g = \tau_0 = 60$ s are chosen too small and therefore make the measurement procedure unsuitable for the measurement purpose since $y^{\#} > y_r$. The choice $\tau_g = \tau_0 = 120$ s would better suit.

Table D.1 — Input data, intermediate values and results of example 1

Input data and specifications			
Quantity	**Symbol**	**Value**	**Standard uncertainty**
Counting measurement, gross effect:			
Number of recorded events	n_g	2 591	
Measurement duration	t_g	360 s	neglected
Counting measurement, background effect:			
Number of recorded events	n_0	41 782	
Measurement duration	t_0	7 200 s	neglected
Ratemeter measurement, gross effect:			
Count rate	r_g	7,2 s^{-1}	
Relaxation time constant	τ_g	60 s	not needed
Ratemeter measurement, background effect:			
Count rate	r_0	5,8 s^{-1}	
Relaxation time constant	τ_0	60 s	not needed
Volume	V with $u(V)$	0,5 l	0,005 l
Detection efficiency	ε with $u(\varepsilon)$	0,3	0,015
Self-absorption factor	f with $u(f)$	0,6	$0{,}4/\sqrt{12}$
Probabilities	α, β, γ	0,05	–
Guideline value	y_r	10 Bq l^{-1}	–

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Table D.1 (*continued*)

Input data and specifications			
Quantity	**Symbol**	**Value**	**Standard uncertainty**
Intermediate values			
Quantity and calculation		**Value** [a]	**Value** [b]
$w = 1/(V\varepsilon f)$ according to Equation (7)		11,11 l^{-1}	
$u_{\text{rel}}^2(w) = u^2(V)/V^2 + u^2(\varepsilon)/\varepsilon^2 + u^2(f)/f^2$ according to Equation (10)		0,039 6	
$\omega = \Phi[y/u(y)]$ according to Equation (E.1)		0,999 9	0,999 4
$p = \omega(1-\gamma/2)$		0,975 0	0,974 4
$q = 1-\omega\gamma/2$		0,975 0	0,975 0
k_p according to Equation (E.2)		1,959 8	1,950 0
k_q according to Equation (E.2)		1,960 0	1,960 2
Results **Measurand**	Y	c_A [a]	c_A [b]
Quantity	**Symbol**	**Value in Bq** l^{-1}	
Primary measurement result	y	15,490 7	15,555 6
Standard uncertainty associated with y	$u(y)$	3,475 5	4,792 3
Decision threshold	y^*	2,377 7	5,683 8
Measurement effect present?	$y > y^*$?	yes	yes
Detection limit	$y^\#$	5,420 2	13,013 7
Measurement procedure suitable?	$y^\# \leqslant y_r$?	yes	no
Lower limit of the confidence interval	$y^\triangleleft$	8,679 1	6,209 3
Upper limit of the confidence interval	$y^\triangleright$	22,302 6	24,949 3
Best estimate of the measurand	$\hat{y}$	15,490 7	15,565 4
Standard uncertainty associated with $\hat{y}$	$u(\hat{y})$	3,475 5	4,776 2

[a] Counting measurement with time preselection.

[b] Ratemeter measurement.

D.3 Example 2: Measurement of the specific activity of a radionuclide after chemical separation

D.3.1 Unknown influence of sample treatment

A sample of solid material containing a radionuclide is examined by chemical separation of this nuclide and subsequent counting measurement of its radiation. The measurand, Y, is the specific activity, a_M (activity of the sample divided by the total mass of the sample, see ISO 31-9) for which the characteristic limits, the best estimate, and the associated standard uncertainty are calculated. The measurement is randomly influenced by sample treatment because of the chemical separation. Therefore, one shall proceed according to B.4. To determine and reduce the influence, several samples of the same kind of material, blanks and also, if necessary, reference samples are separately tested. The results for the respective samples are then averaged and analysed regarding the measurement uncertainty.

The model of the evaluation reads in this case according to Equation (4):

$$Y = A_M = \frac{X_1 - X_2}{X_5 X_7 X_9} = \frac{\overline{r}_g - \overline{r}_0}{M\,\kappa\varepsilon} \qquad \text{(D.2)}$$

$X_1 = \overline{r}_g$ is the mean gross count rate of the samples and $X_2 = \overline{r}_0$ is the mean background count rate of the blanks, $X_5 = M$ is the sample mass assumed here for simplicity to be identical for all samples, blanks and reference samples, $X_7 = \kappa$ is the detection efficiency of the detector used for the counting measurement of the beta radiation in the current measurement geometry, and $X_9 = \varepsilon$ is the chemical yield of chemical separation. There is no formal difference between Equations (D.2) and (D.1), but they shall be distinguished because of the different interpretations of the quantities X_i and, in essence, due to the count rates being averaged or not.

After the counting measurements of the gross effect on m_g samples to be tested and of the background effect on m_0 blanks are carried out with the preselected measurement durations t_g and t_0, respectively, the numbers $\overline{n}_g$ and $\overline{n}_0$ of the recorded events averaged according to Equation (B.7) are available. This first yields the estimates $x_1 = \overline{n}_g / t_g$ and $x_2 = \overline{n}_0 / t_0$ of the respective mean count rates X_1 and X_2 according to Equation (B.8). Moreover, the empirical variances, s_g^2 and s_0^2, of the counting results shall be formed according to Equation (B.7). These yield according to Equation (B.9) the squares of the standard uncertainties $u^2(x_1) = s_g^2/(m_g\, t_g^2)$ and $u^2(x_2) = s_0^2/(m_0 t_0^2)$ associated with the estimates of the count rates. With these results, the estimate, y of the measurand $Y = A_M$, and the associated standard uncertainty, $u(y)$, shall be calculated according to 5.2.2 and, in particular, according to Equations (6) and (9), respectively. $x_3 = 1$ with $u(x_3) = 0$ and $x_4 = 0$ with $u(x_4) = 0$ shall be set since X_3 and X_4 are not involved in the model. Finally, the limits of the confidence interval, the best estimate $\hat{y}$ and the associated standard uncertainty $u(\hat{y})$ can be calculated according to 6.4 and 6.5, in this example as approximations according to Equations (32) and (35) because of $y \geqslant 4u(y)$.

The next step concerns the function $\tilde{u}^2(\tilde{y})$. The standard uncertainty, $u(x_1)$, is not available as a function $h_1(x_1)$. But the interpolation according to Equation (19) can instead be used. However, $\tilde{u}^2(0)$ is needed for this and obtained as follows: setting $y = \tilde{y} = 0$ in Equation (9) first yields $\tilde{u}^2(0) = w^2 \cdot \left[u^2(x_1) + u^2(x_2) \right]$. Moreover, for $\tilde{y} = 0$ according to 5.3.2 and B.4.2, the quotient s_g^2/t_g^2 shall be replaced by s_0^2/t_0^2. This leads with Equation (B.9) to $u^2(x_1) = s_0^2/(m_g\, t_0^2)$ and finally to:

$$\tilde{u}^2(0) = w^2 \cdot (s_0^2 / t_0^2) \cdot (1/m_g + 1/m_0) \tag{D.3}$$

The decision threshold then follows from Equation (21) and the detection limit with the interpolation according to Equation (19) from Equations (22) or (26).

For the input data, specifications, some intermediate values and results, see Table D.2 (the values given in parentheses as well as the results in the last column belong to D.3.2). The guideline value is taken from a directive on monitoring environmental radioactivity.

D.3.2 Known influence of sample treatment

The random influence of sample treatment is sometimes already known from previous measurements, namely from measurements on reference samples or on other samples. The latter should be similar to the current samples and be measured under similar conditions, in order that they can be taken as reference samples although they need not be examined specifically for reference purposes.

One can also proceed in this case according to the equations in B.4.3. For the data of the calculation example, see Table D.2. To enable a comparison, the same input data as in D.3.1 are used here; moreover, the counting results of the reference samples are given in brackets. In contrast to D.3.1, the variance $u^2(x_1)$ according to Equation (B.15) is known as a function $h_1^2(x_1)$. For obtaining $\tilde{u}^2(\tilde{y})$, the estimate y in Equation (B.16) is first replaced by $\tilde{y}$ and then $u^2(x_1)$ and $u^2(x_2)$ by the expressions according to Equations (B.15) and (B.14), respectively. This leads, with $x_1 = \tilde{y}/w + x_2$ and ϑ^2 according to Equation (B.13), to:

$$\tilde{u}^2(\tilde{y}) = w^2 \cdot \left[(x_1/t_g + \vartheta^2 x_1^2)/m_g + (x_2/t_0 + \vartheta^2 x_2^2)/m_0 \right] + \tilde{y}^2 u_{rel}^2(w) \tag{D.4}$$

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The results for D.3.1 and D.3.2 shown in Table D.2 agree in essence, as shall be expected. For the influence parameter ϑ, the value 0,137 7 < 0,2 is acceptable according to B.4.3 results. The decision threshold and the detection limit are in the case of D.3.2 slightly smaller than those of D.3.1.

Table D.2 — Input data, intermediate values and results of example 2

Input data and specifications			
Quantity	**Symbol**	**Value** (in parentheses for D.3.2)	
Number of samples, blanks and reference samples	m_g, m_0, m_r	5, 5, (20)	
Number of recorded events:			
samples (gross effect)	$n_{g,i}$	1 832, 2 259, 2 138, 2 320, 1 649	
blanks (background effect)	$n_{0,i}$	966, 676, 911, 856, 676	
reference samples	$n_{r,i}$	(74 349, 67 939, 88 449, 83 321, 66 657, 64 094, 74 348, 93 576, 56 402, 66 785, 78 194, 69 221, 63 965, 70 503, 74 220, 97 422, 74 476, 71 784, 68 235, 74 989)	
			Standard uncertainty
Measurement durations (general)	t_g, t_0, t_r	30 000 s	neglected
Sample mass (general)	M with $u(M)$	0,100 kg	0,001 kg
Detection efficiency	κ with $u(\kappa)$	0,51	0,02
Chemical yield of ^{90}Sr separation	ε with $u(\varepsilon)$	0,57	0,04
Probabilities	α, β, γ	0,05	–
Guideline value	y_r	0,5 Bq kg^{-1}	–

Intermediate values		
Quantity and calculation	**Symbol**	**Value** (in parentheses for D.3.2)
Mean values	$\overline{n}_g$, $\overline{n}_0$, $\overline{n}_r$	2 039,6; 817,00; (73 946,5)
and empirical standard deviations according to Equation (B.7)	s_g, s_0, s_r	288,14; 134,46; (10 185,0)
Influence parameter according to Equation (B.13)	$\vartheta = \left[(s_r^2 - \overline{n}_r) / \overline{n}_r^2 \right]^{1/2}$	(0,137 7)

Results **Measurand**	Y	A_M (D.3.1)	A_M (D.3.2)
Quantity	**Symbol**	**Value in Bq** kg^{-1}	
Primary measurement result	y	1,401 9	1,401 9
Standard uncertainty associated with y	$u(y)$	0,198 7	0,194 2
Decision threshold	y^*	0,160 4	0,138 4
Measurement effect present?	$y > y^*$?	yes	yes
Detection limit	$y^\#$	0,378 6	0,305 3
Measurement procedure suitable?	$y^\# \leqslant y_r$?	yes	yes
Lower limit of the confidence interval	$y^\triangleleft$	1,012 4	1,021 3
Upper limit of the confidence interval	$y^\triangleright$	1,791 4	1,782 5
Best estimate of the measurand	$\hat{y}$	1,401 9	1,401 9
Standard uncertainty associated with $\hat{y}$	$u(\hat{y})$	0,198 7	0,194 2

D.4 Example 3: Measurement of the activity concentration and of its increase during accumulation on a filter

A radiochemical laboratory is working exclusively with ^{131}I. Due to legal requirements, the activity concentration of the exhaust air shall not exceed the value of 20 Bq m^{-3}. For monitoring compliance with this condition, part of the exhaust air is passed through a filter. The activity of the filter is continuously measured at measurement intervals of duration t with a counting measuring instrument. This implies a case according to B.5. The measurand, Y, of interest is, on the one hand, the activity concentration, $A_{V,j}$, of the exhaust air during the measurement interval, j, (see B.5.2) and, on the other hand, also the increase, $\Delta A_{V,j}$, of the activity concentration, $A_{V,j}$, in comparison with the mean activity concentration, $\overline{A}_{V,j}$, of m preceding measurement intervals (see B.5.3). For each of these cases, the respective characteristic limits, the best estimate and the associated standard uncertainty are to be calculated.

The model for the activity concentration, $A_{V,j}$, is given in Equation (B.19), the model for the increase, $\Delta A_{V,j}$, of the activity concentration in Equation (B.27). They do not differ formally, but merely in the interpretations and approaches of X_2 according to B.5.2 and B.5.3, respectively.

For the input data, specifications, some intermediate values and results, see Table D.3. The numbers n_j from 26 measurement intervals from j = 0 to 25 are available. The measurement interval j = 25 is to be examined. Therefore, m = 24 is set, and only the numbers n_j, for j = 25, 24 and j = 0 are needed, but not explicitly the associated standard uncertainties, $u(n_j) = \sqrt{n_j}$. For the approaches of the values x_1 and $u^2(x_1)$ for X_1 as well as x_2 and $u^2(x_2)$ for X_2, see B.5. The guideline value y_r = 2 Bq m^{-3} is specified for $A_{V,j}$, such that activity concentrations of at least 10 % of the value required by law can still be recognized. For $\Delta A_{V,j}$, the guideline value y_r = 0,2 Bq m^{-3} is chosen, in order that technical measures can be initiated in time for reducing the activity concentration below 10 % of the value required by law. The results are calculated by means of the mentioned models according to Annex A and B.5, especially by application of Equations (B.19) to (B.29). For $Y = A_{V,25}$ in B.5.2, the approximations according to Equations (32) and (35) are used because of $y \geqslant 4u(y)$.

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Table D.3 — Input data, intermediate values and results of example 3

Input data and specifications			
Quantity	**Symbol**	**Value**	**Standard uncertainty**
Number of recorded events in the	$n_j = n_{25}$	15 438	
measurement intervals 25, 24 and 0	$n_{j-1} = n_{24}$	14 356	
(j = 25)	n_0	2 124	
Duration of a measurement interval	t	3 600 s	neglected
Volume	V with $u(V)$	3,00 m^3	0,01 m^3
Calibration factor	ε with $u(\varepsilon)$	0,37	0,02
Probabilities	α, β, γ	0,05	–
Guideline values for $A_{V,j}$ and $\Delta A_{V,j}$	y_r	2,0 and 0,2 Bq m^{-3}	–
Intermediate values			
Quantity and calculation		**Value**	**Standard uncertainty**
x_2 with $u(x_2)$ according to Equation (B.21) for B.5.2		3,987 8 Bq	0,033 3 Bq
Equation (B.29) for B.5.3		4,129 4 Bq	0,034 7 Bq
Results **Measurand**	Y	$A_{V,25}$ (B.5.2)	$\Delta A_{V,25}$ (B.5.3)
Quantity	**Symbol**	**Value in Bq** m^{-3}	
Primary measurement result	y	0,270 8	0,143 2
Standard uncertainty associated with y	$u(y)$	0,045 6	0,044 8
Decision threshold	y^*	0,069 7	0,071 8
Measurement effect present?	$y > y^*$?	yes	yes
Detection limit	$y^\#$	0,141 3	0,145 5
Measurement procedure suitable?	$y^\# \leqslant y_r$?	yes	yes
Lower limit of the confidence interval	$y^\triangleleft$	0,181 4	0,056 0
Upper limit of the confidence interval	$y^\triangleright$	0,360 2	0,231 0
Best estimate of the measurand	$\hat{y}$	0,270 8	0,143 3
Standard uncertainty associated with $\hat{y}$	$u(\hat{y})$	0,045 6	0,044 6

D.5 Examples 4, 5 and 6: Measurement of the specific activity via the intensity of a line on a weakly curved background in a gamma spectrum

D.5.1 Example 4: Measurement using a germanium detector

In the gamma spectrum of a sample recorded by means of a Ge detector, there is a line assigned to the nuclide to be examined and located at channel 927 on a dominant, weakly curved background. The measurand, Y, is the specific activity, A_M, of the sample (activity divided by the total mass of the sample, see ISO 31-9) and shall be calculated from the net intensity (net area) of the line. For this measurand, the characteristic limits, the best estimate and the associated standard uncertainty shall be determined.

Case c) of C.2 is present. As known from energy calibration, the energetic width of a channel amounts to 0,499 5 keV, and the energetic full width at half-maximum of the line is 2,0 keV. This corresponds to a full width at half-maximum of h = 4,00 channels. According to Equation (C.10), $t_g \approx 1{,}2\ h = 4{,}8$ is set as the width

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of region B. The region of channels 925 to 929 with the width t_g = 5 and located symmetrically to channel 927 is therefore specified as region B (see Figure C.1). This region thus covers in this case approximately the portion f = 86 % of the line area [see below Equation (C.10)].

For each of the four regions A_i bordering region B on both sides for the determination of the weakly curved background, the width t = 13 is chosen according to C.3. The total width thus amounts to t_0 = 52. This width cannot be enlarged since there is another possible line at channel 958 with the same full width at half-maximum and therefore located in channels 956 to 960. Thus, at most the 26 channels 930 to 955 remain for the regions A_3 and A_4.

For the input data, specifications, some intermediate values and results, see Table D.4. The results are calculated on the basis of the following model according to Annex A and C.2. Especially, Equations (C.3), (C.4), (C.5), (C.10) and (C.12) are used. The model reads:

$$Y = A_M = \frac{X_1 - X_2}{X_5 X_7 X_9 X_{11} X_{13}} = \frac{X_g - Z_0}{T f M \varepsilon i} \tag{D.5}$$

$X_1 = X_g$ is the estimator of the gross effect in region B, $X_2 = Z_0$ is the estimator of the background effect, i.e. of the background contribution to the line in region B, and $X_5 = T$ is the measurement duration. The correction factor $X_7 = f$ takes into account that region B does not completely cover the line in case of a dominant background. For f, see above and Equation (C.10). The standard uncertainty of f is neglected because f, if necessary, can be calculated exactly to an arbitrary number of digits. Moreover, $X_9 = M$ is the sample mass, $X_{11} = \varepsilon$ is the detection efficiency of the detector measured with f = 1, and $X_{13} = i$ is the photon emission probability of the gamma line. The values of M and ε and the associated standard uncertainties $u(M)$ and $u(\varepsilon)$ were determined in previous investigations. The value of i and the associated standard uncertainty, $u(i)$, are taken from a tabular compilation of decay data of radioactive nuclides. The guideline value, y_r, is specified by a directive on monitoring of environmental radioactivity.

For X_1, the values $x_1 = n_g$ and $u^2(x_1) = n_g$ are set (see C.1 and F.1). It should be noted here that $X_1 = X_g$ does not estimate a count rate, but instead the parameter of a Poisson distribution. Therefore, the measurement duration T appears in the denominator of Equation (D.5). For the values z_0 and $u^2(z_0)$ for $X_2 = Z_0$, see Equation (C.12).

D.5.2 Example 5: Measurement using a sodium iodide detector

Figure C.1 shows a section of a gamma spectrum recorded using a NaI detector. There is a line of interest located with its centre, $\bar{\vartheta}_g$, at channel 500 on a non-dominant, weakly curved background. The measurand, Y, is the net intensity, I (net area), of the line. For this measurand, the characteristic limits, the best estimate and the associated standard uncertainty shall also be determined.

Again, case c) of C.2 is present. The full width at half-maximum of the line amounts to $h = \sigma\sqrt{8 \ln 2} = 32{,}45$ channels as a result of example 6 in D.5.3. Thus, $t_g \approx 2{,}5\ h \approx 81$ shall be set as the width of region B according to Equation (C.9). Therefore, the region of channels 461 to 539 with the width t_g = 79 and located symmetrically to channel 500 is specified as region B (see Figure C.1). This region thus covers in this case almost f = 100 % of the line area.

For each of the four regions A_i bordering region B on both sides for the determination of the weakly curved background, the width t = 21 is chosen according to C.3. The total width thus amounts to $t_0 = 4t$ = 84. This width cannot be enlarged because of the increasing background below channel 419 and above channel 581 caused by neighbouring lines as shown in Figure C.1.

For the multi-channel spectrum data and other input data, specifications, some intermediate values and results, see Tables D.4 and D.5. The results are calculated on the basis of the following model as in example 4. The model here has a simpler form and reads

$$Y = I = X_1 - X_2 = X_g - Z_0 \tag{D.6}$$

so that w = 1 and $u_{rel}(w)$ = 0. For the input quantities $X_1 = X_g$ and $X_2 = Z_0$, see also example 4. A guideline value is not specified. Because $y \geqslant 4u(y)$ in the present case, the approximations according to Equations (32) and (35) are used.

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As shown in Figure C.1, both a straight line with m = 2 [case b)] and a cubic parabola with m = 4 [case c)] are adjusted to the spectrum background in the regions A_i according to C.3. In the case of the straight line, the regions A_1 and A_2 are combined, as well as the regions A_3 and A_4. With $M = t_0 = 84$ and $\delta = 0{,}05$ and according to Equation (C.14), the standardized chi-square $\chi^2_s = \left|\chi^2 - M + m\right| \Big/ \sqrt{2(M-m)} = 2{,}71 > k_{1-\delta/2} = 1{,}96$ follows for the straight line, while for the parabola the standardized chi-square $\chi^2_s = 0{,}41 < k_{1-\delta/2} = 1{,}96$ is obtained. The straight line therefore cannot be accepted because the chi-square condition is not fulfilled.

Table D.4 — Input data, intermediate values and results of examples 4, 5 and 6

Input data and specifications of example 4			
Quantity	**Symbol**	**Value**	**Channels**
Energetic channel width		0,499 5 keV	
Energetic full width at half-maximum of the line		2,0 keV	
Number of recorded events in			
region A_1	n_1	3 470	899 to 911
region A_2	n_2	3 373	912 to 924
region B	n_g	1 440	925 to 929
region A_3	n_3	3 343	930 to 942
region A_4	n_4	3 208	943 to 955
Width of region A_i	t	13	
Width of region B	t_g	5	
			Standard uncertainty
Measurement duration	T	21 600 s	neglected
Correction factor	f	0,858 5	neglected
Sample mass	M with $u(M)$	1,000 kg	0,001 kg
Detection efficiency	ε with $u(\varepsilon)$	0,060	0,004
Photon emission probability	i with $u(i)$	0,98	0,02
Probabilities	α, β, γ	0,05	–
Guideline value	y_r	0,5 Bq kg^{-1}	–

Input data and specifications of examples 5 and 6				
Quantity		**Symbol**	**Value**	**Channels, comments**
Full width at half-maximum of the line		h	32,45	result of example 6
Number of recorded events in				
region A_1	A_1 for straight line	n_1	17 326	419 to 439
region A_2		n_2	17 291	440 to 460
region B		n_g	84 221	461 to 539
region A_3	A_2 for straight line	n_3	12 069	540 to 560
region A_4		n_4	11 434	561 to 581
Width of region A_i		t	21	
Width of region B		t_g	79	
Probabilities		α, β, γ, δ	0,05	
Guideline value		y_r	–	not specified

Table D.4 (*continued*)

Intermediate values		**Example 4**	**Example 5**	
Quantity and calculation		**Value**	**Value**	
$n_0 = n_1 + n_2 + n_3 + n_4$		13 394	58 120	
$n_0' = n_1 - n_2 - n_3 + n_4$		–38	–600	
Total width $t_0 = 4t$ of the regions A_i		52	84	
Background contribution z_0 with standard		1 293,2	56 120	
uncertainty $u(z_0)$ according to Equation (C.12)		19,7	631	
Intermediate values of example 6				
Quantity and calculation	**Symbol**	**Value**	**Standard uncertainty**	
Standard deviation of the line by minimizing χ^2_s	σ	13,78	not determined	
Unfolding parameters y_k with	$y_1 = y$	29 550,3	369,7	
standard uncertainties $u(y_k)$	y_2	–35,44	15,36	
according to Equations	y_3	694,7	5,25	
(C.32) to (C.34) and (C.36)	y_4	–4,035	0,576	
	y_5	$-1{,}71\times10^{-3}$	$1{,}45\times10^{-3}$	
	y_6	$2{,}60\times10^{-4}$	$5{,}80\times10^{-5}$	
Results		**Example 4**	**Example 5**	**Example 6**
Measurand	Y	A_M	I	I
Quantity	**Symbol**	value in Bq kg^{-1}	unit 1	unit 1
Primary measurement result	y	0,134 6	28 100	29 550
Standard uncertainty associated with y	$u(y)$	0,040 3	695	370
Decision threshold	y^*	0,061 9	1 109	488
Measurement effect present?	$y > y^*$?	yes	yes	yes
Detection limit	$y^\#$	0,127 9	2 220	980
Measurement procedure suitable?	$y^\# \leqslant y_r$?	yes	–	–
Lower limit of the confidence interval	$y^\triangleleft$	0,055 8	26 739	28 826
Upper limit of the confidence interval	$y^\triangleright$	0,213 7	29 462	30 275
Best estimate of the measurand	$\hat{y}$	0,134 7	28 100	29 550
Standard uncertainty associated with $\hat{y}$	$u(\hat{y})$	0,040 2	695	370
Standardized chi-square	χ^2_s	–	0,41 (parabola) 2,71 (straight line)	0,78
Chi-square condition fulfilled?	$\chi^2_s \leqslant k_{1-\delta/2}$	–	yes (parabola) no (straight line)	yes

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Table D.5 — Multi-channel spectrum data of examples 5 and 6

A_1		A_2		B		B		B		A_3		A_4	
i	x_i	i	x_i	i	x_i	i	x_i	i	x_i	i	x_i	i	x_i
419	872	440	817	461	850	487	1 219	513	1 250	540	584	561	570
420	867	441	817	462	807	488	1 301	514	1 164	541	604	562	543
421	830	442	792	463	817	489	1 401	515	1 146	542	579	563	519
422	865	443	804	464	797	490	1 399	516	1 119	543	548	564	495
423	822	444	788	465	795	491	1 346	517	1 078	544	559	565	564
424	787	445	815	466	811	492	1 452	518	1 049	545	588	566	554
425	812	446	854	467	827	493	1 426	519	1 010	546	617	567	566
426	799	447	817	468	784	494	1 430	520	956	547	576	568	543
427	860	448	875	469	829	495	1 550	521	920	548	607	569	533
428	832	449	857	470	872	496	1 503	522	901	549	580	570	540
429	807	450	773	471	855	497	1 486	523	880	550	585	571	572
430	823	451	828	472	868	498	1 561	524	823	551	599	572	546
431	838	452	850	473	895	499	1 501	525	782	552	598	573	549
432	833	453	812	474	965	500	1 611	526	745	553	606	574	553
433	795	454	818	475	888	501	1 471	527	703	554	555	575	528
434	806	455	872	476	915	502	1 608	528	742	555	572	576	585
435	815	456	804	477	887	503	1 551	529	690	556	566	577	560
436	793	457	865	478	1 002	504	1 545	530	721	557	545	578	518
437	837	458	820	479	1 008	505	1 403	531	684	558	501	579	567
438	807	459	792	480	1 064	506	1 486	532	683	559	529	580	509
439	826	460	821	481	1 033	507	1 464	533	678	560	571	581	520
				482	1 110	508	1 365	534	680				
				483	1 131	509	1 371	535	609				
				484	1 160	510	1 341	536	575				
				485	1 264	511	1 305	537	614				
				486	1 194	512	1 292	538	624				
								539	579				

i Channel number

x_i Counts recorded in channel i

A_k Channel regions for the background determination

B Channel regions of the line

D.5.3 Example 6: Unfolding a gamma spectrum

The multi-channel gamma spectrum evaluated in example 5 and shown in Figure C.1 is also linearly unfolded according to Equations (C.32) to (C.34) and (C.36) with the same input data listed in Tables D.4 and D.5. This makes feasible a direct comparison of applying the two methods. The results are also shown in Table D.4 and Figure C.1.

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The n = 6 fitting functions given in Equation (C.36) are used to form the spectrometer response matrix $\boldsymbol{A}$. The channel number i is taken as E, the energy scale. The standard deviation, σ, of the line in question and the parameter, a, of the arctan step function are not given. Therefore, a is first identified with σ, then a primary value of σ estimated by eye is varied in repeated linear unfoldings until the standardized chi-square χ^2_s becomes a minimum. The value of σ obtained in this way is also used in example 5 for the full width at half-maximum $h = \sigma\sqrt{8\ln 2}$.

The estimates, x_i, of the input quantities, X_i, are the counts recorded in the m = 163 individual channels 419 to 581 of the multi-channel spectrum (see Table D.5). They form the column matrix $\boldsymbol{x} = (x_1, ..., x_m)^T$. Moreover, $u^2(x_i) = x_i$ and $u(x_i,x_j) = 0$ $(i \neq j)$ by assuming Poisson statistics and uncorrelated counting in different channels. This yields the diagonal uncertainty matrix, $\boldsymbol{U}_{\boldsymbol{x}}(\boldsymbol{x}) = \mathrm{diag}(\boldsymbol{x})$. The n = 6 measurand estimates y_k to be calculated are values of the coefficients Y_k of the fitting functions according to Equation (C.36) and form the column matrix $\boldsymbol{y} = (y_1, ..., y_6)^T$. The measurand, Y, of interest is the net line intensity Y_1 as in example 5. Thus, $y = y_1$. The model matrix equation of the unfolding is $\boldsymbol{x} = \boldsymbol{A}\boldsymbol{y}$. The measurands, Y_k, turn out to be correlated, but only the standard uncertainties $u(y_k)$ associated with the results, y_k, are listed in Table D.4; the associated correlation coefficients are dispensed with.

The two measurand results $y = y'$ and $y = y''$ of examples 5 and 6 differ considerably. Whether or not the difference is actually significant can be answered as follows: the difference $z = y' - y''$ of two independently determined estimates, y' and y'', of the same measurand is an estimate of the quantity Z with the true value 0. This value 0 should then be contained in the confidence interval between the limits $z \pm k_{1-\gamma/2} \cdot u(z)$ with $u(z) = \sqrt{u^2(y') + u^2(y'')}$. This leads to the condition $|z| / u(z) \leqslant k_{1-\gamma/2}$. Accordingly, with $\gamma = 0{,}05$ the two results obtained by the two distinct methods of example 5 and 6 cannot be taken as significantly different since $|z| / u(z) = 1{,}84 < 1{,}96$ proves true.

The standard uncertainties, $u(y)$, and the characteristic limits of examples 5 and 6 also differ considerably. This can be due to the fact that in example 6 the full spectrum information is taken into account whereas in example 5 only counts summed up over the spectrum regions are used. However, the unfolded background in region B of the spectrum nearly coincides with the (not accepted) straight-line approximation of example 5 (see Figure C.1). The reason for that can be the fact that the arctan step function barely plays a part.

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Annex E
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Distribution function of the standardized normal distribution

The distribution function of the standardized normal distribution is defined by Equation (E.1):

$$\Phi(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{t} \exp\left(-\frac{v^2}{2}\right) \mathrm{d}v = \frac{1}{2} + \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{t^2}{2}\right) \sum_{j=0}^{\infty} \frac{t^{2j+1}}{1 \cdot 3 \cdots (2j+1)} \tag{E.1}$$

and its quantile k_p for the probability p by $\Phi(k_p) = p$ (see Reference [29]). The second expression in Equation (E.1) can serve for the numerical calculation of $\Phi(t)$. The series in Equation (E.1) converges for every t. Values of $\Phi(t)$ are presented in Table E.1. The relations $\Phi(-t) = 1 - \Phi(t)$ and $k_{1-p} = -k_p$ apply.

The quantile k_p of the standardized normal distribution can be calculated numerically as follows using the Newton iteration procedure: with an approximation t for k_p, an improved approximation t' results from Equation (E.2):

$$t' = t + \sqrt{2\pi} \exp(t^2/2)\left[p - \Phi(t)\right] \tag{E.2}$$

The value $t = 0$ can be chosen as a starting approximation.

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Table E.1 — Distribution function $\Phi(t)$ of the standardized normal distribution

t	$\Phi(t)$	t	$\Phi(t)$	t	$\Phi(t)$	t	$\Phi(t)$	t	$\Phi(t)$
0,00	0,500 0	0,60	0,725 8	1,20	0,884 9	1,80	0,964 1	2,40	0,991 8
0,02	0,508 0	0,62	0,732 4	1,22	0,888 8	1,82	0,965 6	2,42	0,992 2
0,04	0,516 0	0,64	0,738 9	1,24	0,892 5	1,84	0,967 1	2,44	0,992 7
0,06	0,523 9	0,66	0,745 4	1,26	0,896 1	1,86	0,968 6	2,46	0,993 0
0,08	0,531 9	0,68	0,751 8	1,28	0,899 7	1,88	0,970 0	2,48	0,993 4
0,10	0,539 8	0,70	0,758 0	1,30	0,903 2	1,90	0,971 3	2,50	0,993 8
0,12	0,547 8	0,72	0,764 2	1,32	0,906 6	1,92	0,972 6	2,52	0,994 1
0,14	0,555 7	0,74	0,770 4	1,34	0,909 9	1,94	0,973 8	2,54	0,994 5
0,16	0,563 6	0,76	0,776 4	1,36	0,913 1	1,96	0,975 0	2,56	0,994 8
0,18	0,571 4	0,78	0,782 3	1,38	0,916 2	1,98	0,976 2	2,58	0,995 1
0,20	0,579 3	0,80	0,788 1	1,40	0,919 2	2,00	0,977 2	2,60	0,995 3
0,22	0,587 1	0,82	0,793 9	1,42	0,922 2	2,02	0,978 3	2,62	0,995 6
0,24	0,594 8	0,84	0,799 6	1,44	0,925 1	2,04	0,979 3	2,64	0,995 9
0,26	0,602 6	0,86	0,805 1	1,46	0,927 8	2,06	0,980 3	2,66	0,996 1
0,28	0,610 3	0,88	0,810 6	1,48	0,930 6	2,08	0,981 2	2,68	0,996 3
0,30	0,617 9	0,90	0,815 9	1,50	0,933 2	2,10	0,982 1	2,70	0,996 5
0,32	0,625 5	0,92	0,821 2	1,52	0,935 7	2,12	0,983 0	2,72	0,996 7
0,34	0,633 1	0,94	0,826 4	1,54	0,938 2	2,14	0,983 8	2,74	0,996 9
0,36	0,640 6	0,96	0,831 5	1,56	0,940 6	2,16	0,984 6	2,76	0,997 1
0,38	0,648 0	0,98	0,836 5	1,58	0,943 0	2,18	0,985 4	2,78	0,997 3
0,40	0,655 4	1,00	0,841 3	1,60	0,945 2	2,20	0,986 1	2,80	0,997 4
0,42	0,662 8	1,02	0,846 1	1,62	0,947 4	2,22	0,986 8	2,90	0,998 1
0,44	0,670 0	1,04	0,850 8	1,64	0,949 5	2,24	0,987 4	3,00	0,998 6
0,46	0,677 2	1,06	0,855 4	1,66	0,951 5	2,26	0,988 1	3,10	0,999 0
0,48	0,684 4	1,08	0,859 9	1,68	0,953 5	2,28	0,988 7	3,20	0,999 3
0,50	0,691 5	1,10	0,864 3	1,70	0,955 4	2,30	0,989 3	3,30	0,999 5
0,52	0,698 5	1,12	0,868 6	1,72	0,957 3	2,32	0,989 8	3,40	0,999 7
0,54	0,705 4	1,14	0,872 9	1,74	0,959 1	2,34	0,990 4	3,50	0,999 8
0,56	0,712 3	1,16	0,877 0	1,76	0,961 0	2,36	0,990 9	3,60	0,999 8
0,58	0,719 0	1,18	0,881 0	1,78	0,962 5	2,38	0,991 3	3,80	0,999 9
								$\geqslant$ 4,00	1,000 0

NOTE $k_p = t$ is the quantile for the probability $p = \Phi(t)$. The relations $\Phi(-t) = 1-\Phi(t)$ and $k_{1-p} = -k_p$ apply.

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Annex F
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Explanatory notes

F.1 General aspects of counting measurements

A measurement of ionizing radiation consists in general, at least partially, in counting electronic pulses induced by ionizing radiation events. Such a measurement comprises several individual countings, but can also comprise sequences of individual countings. Examples are the countings on samples of radioactive material or on blanks, countings for the determination of the background effect or the countings in the individual channels of a multi-channel spectrum or in a temporal sequence in the same measurement situation. With each of the countings, either the measurement duration (time preselection) or the counting result (preselection of counts) can be fixed. On the basis of Bayesian statistics, all countings are treated in the same way as follows (see Reference [17]).

The pulse number, N, of each of the countings is taken as a separate random variable. n is the counting result and t is the counting duration (measurement duration). N has the expectation value $\tilde{r} \cdot t$, where $\tilde{r}$ is the count rate or, with spectrum measurements, the spectral density. In the latter case, t is the channel width with respect to the assigned quantity, for instance, the particle energy. Either $\tilde{r}$ or $\tilde{r} \cdot t$ is the measurand. It is assumed that dead-time and mean-life effects, pile-up of the pulses, and instrumental instabilities can be neglected during counting and that all the counted pulses are induced by different ionizing radiation events which are physically independent. The pulse number, N, follows a Poisson distribution and the pulse numbers of all the countings are independent of each another.

Irrespective of whether n pulses are recorded in a measurement of a preselected duration (or of a fixed channel width), t (time preselection), or whether the measurement duration, t, needed for the counting of a preselected pulse number, n, is measured (preselection of counts), $\tilde{r} \cdot t$ follows a gamma distribution (see References [38,39]), where $\tilde{r}$ is taken as a random variable. Then the best estimate, r, of the count rate (or spectral density) and the standard uncertainty, $u(r)$, associated with r follow from:

$$r = \mathrm{E}(\tilde{r}) = n/t \;\; ; \;\; u^2(r) = \mathrm{Var}(\tilde{r}) = n/t^2 = r/t \tag{F.1}$$

The case n = 0 results in $u(r)$ = 0. This disappearing uncertainty of $\tilde{r}$ means that $\tilde{r} = 0$ is exactly valid. But $u(r)$ = 0 is an unrealistic result because, with a finite measurement duration, one can never be sure that exactly $\tilde{r} = 0$ if no pulse happens to be recorded. This case can also lead to a zero denominator when the least-squares method according to ISO/IEC Guide 98-3 (see References [1, 2]) is applied and a division by $u^2(r)$ shall be made. This shortcoming, e.g. in low-level measurements, can be avoided by replacing all of the counting results n by n + 1 or, with a multi-channel spectrum, by a suitable combination of channels. Here, the measurement duration (or channel width) is assumed to be chosen from experience such that at least a few pulses can be expected if $\tilde{r} > 0$.

F.2 Bayesian statistics in measurement

F.2.1 Special quantities and symbols used in this Clause

$f(y|\tilde{y})$ probability distribution; i.e. the conditional distribution of estimates, y, given the true value, $\tilde{y}$, of the measurand, Y

$f(\tilde{y}|y)$ probability distribution of the true value, $\tilde{y}$, of the measurand, Y, given the measured estimate, y (Bayesian statistics)

$f_0(\tilde{y}|y)$ likelihood; it is the probability distribution that the measurand, Y, has the true value, $\tilde{y}$, if only the measured value, y, and the associated uncertainty, $u(y)$, are given

$f(\tilde{y})$ model prior; it represents all the information about the measurand available before the experiment is performed

F.2.2 Probability distributions

Based on Bayesian statistics (see Reference [8]) and the Bayesian theory of measurement uncertainty (see References [6, 7, 16, 17]), characteristic limits such as the decision threshold, detection limit and limits of a confidence interval can be calculated taking into account all sources of uncertainty. This approach consists of the complete evaluation of a measurement according to ISO/IEC Guide 98-3 and the succeeding determination of the characteristic limits by using the standard uncertainty obtained from the evaluation. Bayesian statistics allows a consistent foundation of ISO/IEC Guide 98-3 for both type A and type B uncertainties. This is in contrast to conventional (frequentistic) statistics in which type B uncertainties cannot be accounted for.

The basic difference between conventional and Bayesian statistics lies in the different use of the term probability. Considering measurements, conventional statistics describes the probability distribution, $f(y|\tilde{y})$, i.e. the conditional distribution of estimates, y, given the true value, $\tilde{y}$, of the measurand, Y. Since the true value of a measurand is principally unknown, it is the basic task of an experiment to make statements about it. Bayesian statistics allows the calculation of the probability distribution, $f(\tilde{y}|y)$, of the true value, $\tilde{y}$, of the measurand, Y, given the measured estimate, y. The measurement uncertainty and the characteristic limits are based on the distributions, $f(y|\tilde{y})$ and $f(\tilde{y}|y)$. These implicitly depend on further conditions and information such as the model, measurement data and associated uncertainties.

In order to establish $f(\tilde{y}|y)$, one uses an approach which separates the information about the measurand obtained from the actual experiment from other information available about the measurand by

$$f(\tilde{y}|y) = C \cdot f_0(\tilde{y}|y) \cdot f(\tilde{y}) \tag{F.2}$$

$f_0(\tilde{y}|y)$, called the likelihood, is the probability distribution that the measurand, Y, has the true value, $\tilde{y}$, if only the measured value, y, and the associated uncertainty, $u(y)$, are given. It only accounts for the measured values and neglects any other information about the measurand. $f(\tilde{y})$, called the model prior, represents all the information about the measurand available before the experiment is performed. Therefore, it does not depend on y. C is a normalization constant.

If, for instance, an activity of a radiation source or a concentration of an element is the measurand, there exists the meaningful information that the measurand is non-negative ($\tilde{y} \geqslant 0$) before the measurement is carried out. This yields for $f(\tilde{y})$:

$$f(\tilde{y}) = \begin{cases} \text{const} & (\tilde{y} \geqslant 0) \\ 0 & (\tilde{y} < 0) \end{cases} \tag{F.3}$$

Note that the actual result, y, of a measurement, for instance a net count rate, can be negative. But the experimentalist knows a priori without performing an experiment that the true value, $\tilde{y}$, is non-negative. All non-negative values of the measurand have the same a priori probability, if there is no other information available about the true value before the measurement has been performed.

Since the likelihood, $f_0(\tilde{y}|y)$, in essence considers the experimental information, the expectation, $\mathrm{E}_0(\tilde{y}|y) = y$, and the variance, $\mathrm{Var}_0(\tilde{y}|y) = u^2(y)$, should hold true for the probability distribution, $f_0(\tilde{y}|y)$.

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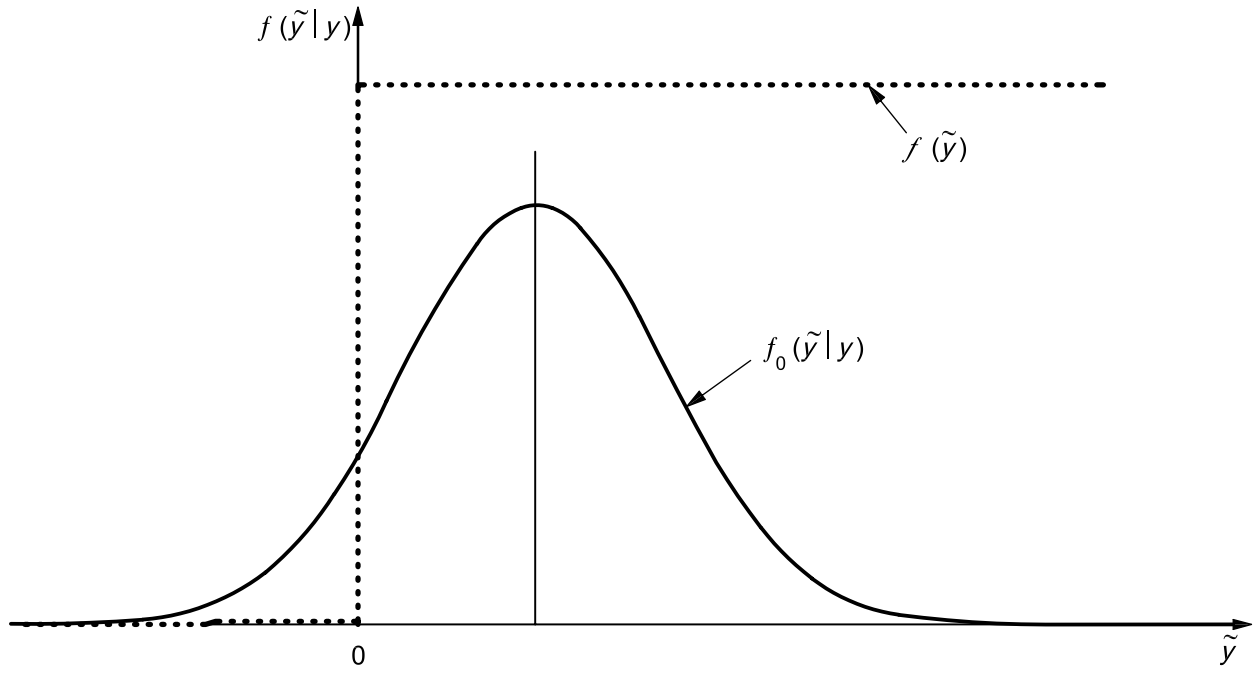
According to References [6, 16], the probability distribution, $f(\tilde{y}|y)$, can be determined by applying the principle of maximum (information) entropy S (see Reference [17]):

$$S = -\int f_0(\tilde{y}|y) \cdot f(\tilde{y}) \cdot \ln\left[f_0(\tilde{y}|y) \right] \mathrm{d}\tilde{y} = \max \tag{F.4}$$

Equation (F.4) can be solved with the constraints $\mathrm{E}_0(\tilde{y}|y) = y$ and $\mathrm{Var}_0(\tilde{y}|y) = u^2(y)$ obtained with the likelihood, $f_0(\tilde{y}|y)$, by the method of Lagrangian multiplicators and one obtains the result:

$$f(\tilde{y}|y) = C \cdot f(\tilde{y}) \cdot \exp\left\{ -(\tilde{y} - y)^2 \Big/ \left[2 \cdot u^2(y) \right] \right\} \tag{F.5}$$

Accordingly, the distribution $f(\tilde{y}|y)$ is a product of the model prior and a Gaussian N[y,$u(y)$], i.e. a truncated Gaussian (Figure F.1). Note that the Gaussian in Equation (F.5) is not an approximation as in conventional statistics or a distribution of measured values from repeated or counting measurements. It is instead the explicit result of maximizing the information entropy and expresses the state of knowledge about the measurand, Y.



Key

$\tilde{y}$ true value of the measurand, Y

$f(\tilde{y}|y)$ probability distribution of the true value, $\tilde{y}$, of the measurand, Y, given the measured estimate, y

For the curves, see the text.

Figure F.1 — Illustration of the probability distribution given in Equation (F.5) for a non-negative measurand Y

After $f(\tilde{y}|y)$ is obtained, the Bayes theorem also allows the calculation of the probability distribution, $f(y|\tilde{y})$, of an estimate, y, given the true value, $\tilde{y}$, of the measurand, Y:

$$f(y|\tilde{y}) \cdot f(\tilde{y}) = f(\tilde{y}|y) \cdot f(y) \tag{F.6}$$

The distribution, $f(y)$, is uniform for all possible measurement results, y, before the measurement is carried out and $f(\tilde{y})$ is uniform for all $\tilde{y} \geqslant 0$ according to Equation (F.3). Thus, $f(y|\tilde{y})$ is obtained from Equations (F.5) and (F.6) by approximating the now not available $u(y)$ by a function $\tilde{u}(\tilde{y})$.

$$f(y|\tilde{y}) = C \cdot \exp\left\{-(y-\tilde{y})^2 \Big/ \left[2 \cdot \tilde{u}^2(\tilde{y})\right]\right\} \quad (\tilde{y} \geqslant 0) \tag{F.7}$$

The probability distribution, $f(y|\tilde{y})$, is a Gaussian for a given true value, $\tilde{y}$, of the measurand, Y, with the standard uncertainty, $\tilde{u}(\tilde{y})$. Note, that the true value, $\tilde{y}$, is now a parameter in Equation (F.7) and that the variance, $u^2(y)$, of the probability distribution, $f(\tilde{y}|y)$, is expressed by the variance, $\tilde{u}^2(\tilde{y})$, of the probability distribution, $f(y|\tilde{y})$:

$$u^2(y) = \tilde{u}^2(\tilde{y}) \tag{F.8}$$

F.2.3 Calculation of the standard uncertainty as a function of the true value of the measurand

For the provision and numerical calculation of the decision threshold and detection limit, the standard uncertainty of the measurand is needed as a function $\tilde{u}(\tilde{y})$ of the true value, $\tilde{y} \geqslant 0$ of the measurand. This function shall be determined in a way similar to $u(y)$ within the framework of the evaluation of the measurements by application of ISO/IEC Guide 98-3:2008 (see References [1, 2]). In most cases, $\tilde{u}(\tilde{y})$ shall be formed as a positive square root of a variance function, $\tilde{u}^2(\tilde{y})$, calculated first with $f(y|\tilde{y})$:

$$\tilde{u}^2(\tilde{y}) = \mathrm{Var}(y|\tilde{y}) \tag{F.9}$$

This function shall be defined, unique and continuous for all $\tilde{y} \geqslant 0$ and shall not assume negative values. In some cases, $\tilde{u}(\tilde{y})$ can be explicitly specified, provided that $u(x_1)$ is given as a function $h_1(x_1)$ of x_1. In such cases, y shall be replaced by $\tilde{y}$ and Equation (2) shall be solved for the estimate x_1 of the input quantity, X_1, which in the following is always taken as the gross effect quantity. With a specified $\tilde{y}$, the value x_1 can also be calculated numerically from Equation (2), for instance, by means of an iteration procedure, which results in x_1 as a function of $\tilde{y}$ and x_2, ..., x_m. This function shall replace x_1 in Equation (3) and in $u(x_1) = h_1(x_1)$, which finally yields $\tilde{u}(\tilde{y})$ instead of $u(y)$. In most cases of the models dealt with in this International Standard, one shall proceed in this way. Otherwise, $\tilde{u}(\tilde{y})$ can be obtained as an approximation by interpolation from the data, y_j and $u(y_j)$, of several measurements; see Equation (19) and Figure (F.2).

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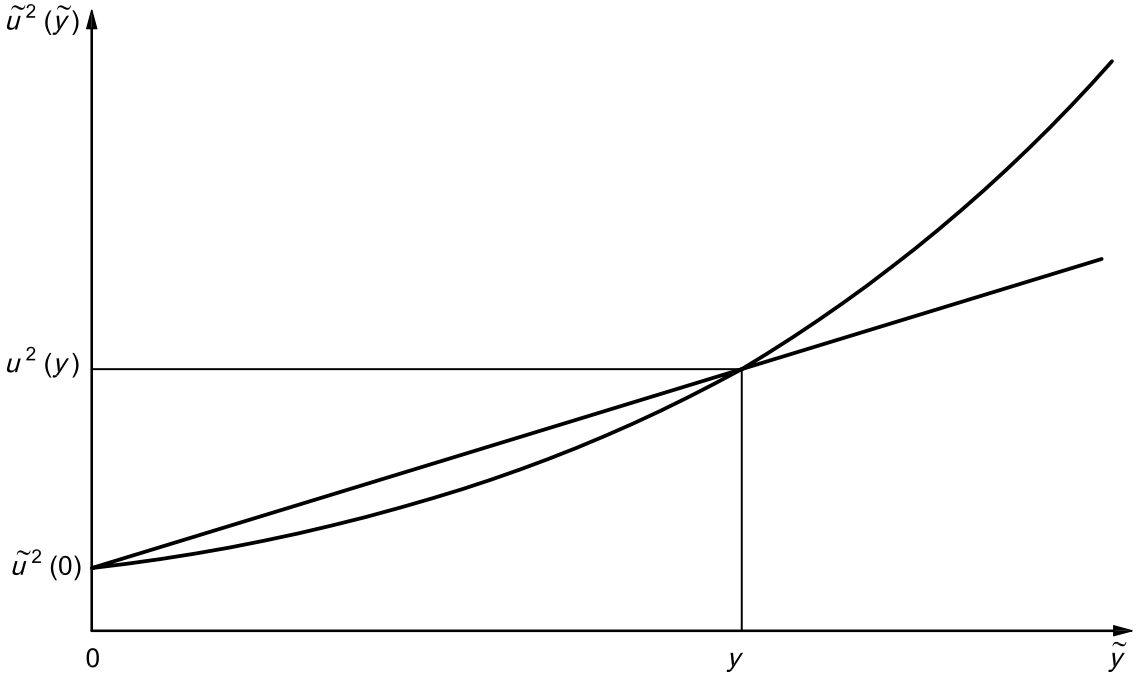

Key

$\tilde{y}$ true value of the measurand, Y

$\tilde{u}^2(\tilde{y})$ variance of the probability distribution $f(y|\tilde{y})$

For the other symbols, see text.

Figure F.2 — Illustration of the function $\tilde{u}^2(\tilde{y})$ and the interpolation formula of Equation (19)

F.2.4 Decision threshold and detection limit

Without a detailed mathematical foundation of Bayesian characteristic limits, which can be found elsewhere (see Reference [17]), the characteristic limits can now be defined for a non-negative measurand, Y, which is, for instance, a concentration of an element or an activity of a radionuclide in a sample. The true value, $\tilde{y}$, is zero if the element or the radionuclide is not present.

For the determination of the decision threshold and the detection limit, the standard uncertainty, $\tilde{u}(\tilde{y})$, as a function of the true value, $\tilde{y}$, of the measurand shall be calculated if possible. Otherwise, approximate solutions as described in 5.3.3 and 6.3 are to be used.

Then, the decision threshold y^* (Figure F.3) is a characteristic limit, which when exceeded by a result, y, of a measurement, one decides that the element or radionuclide is present in the sample. If $y \leqslant y^*$, a true value of zero is sufficiently probable and one decides that the element or radionuclide is not found in this sample. If the decision rule

$$P(y > y^* | \tilde{y} = 0) = \int_{y^*}^{\infty} f(y | \tilde{y} = 0)\, \mathrm{d}y = \alpha \tag{F.10}$$

is observed, a wrong decision is made with the probability α.

The decision threshold is given by:

$$y^* = k_{1-\alpha} \cdot \tilde{u}(0) \tag{F.11}$$

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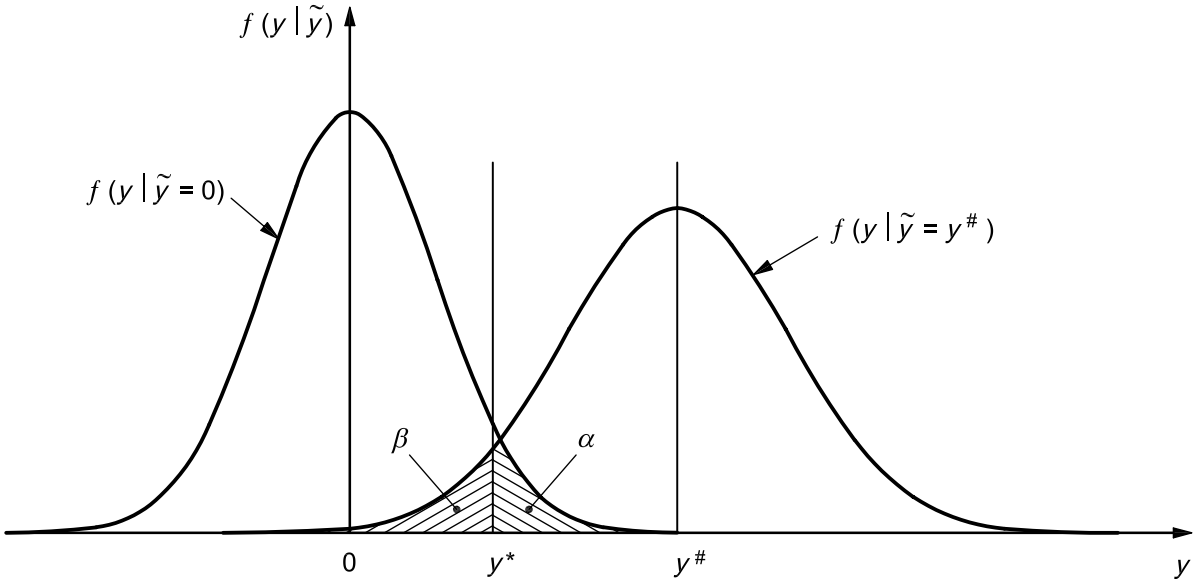
with $k_{1-\alpha}$ being the (1–α)-quantile of the standardized normal distribution. $\tilde{u}(0)$ is the uncertainty of the measurand if its true value, $\tilde{y}$, equals zero.

The detection limit, $y^{\#}$, (Figure F.3) is the smallest true value of the measurand detectable with the measuring method. It is defined by

$$P(y < y^* | \tilde{y} = y^{\#}) = \int_{-\infty}^{y^*} f(y | \tilde{y} = y^{\#})\, \mathrm{d}y = \beta \tag{F.12}$$



Key

y	primary measurement result of the measurand, Y
$f(y\|\tilde{y})$	probability distribution (conditional distribution of estimates, y, given the true value, $\tilde{y}$, of the measurand, Y)

For the other symbols and the curves, see text.

Figure F.3 — Decision threshold y^* and detection limit $y^{\#}$

The detection limit, $y^{\#}$, is sufficiently larger than the decision threshold, y^*, so that the probability of $y < y^*$ with the consequence to wrongly decide that the physical effect is not present, equals the probability β. The detection limit is given by:

$$y^{\#} = y^* + k_{1-\beta} \cdot \tilde{u}(y^{\#}) \tag{F.13}$$

with $k_{1-\beta}$ being the (1–β)-quantile of the standardized normal distribution.

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F.2.5 Limits of the confidence interval and best estimate

The confidence interval (Figure F.4) includes for a result, y, of a measurement which exceeds the decision threshold, y^*, the true value of the measurand with a probability $1-\gamma$. It is enclosed by the lower and upper limit of the confidence interval, respectively $y^{\triangleleft}$ and $y^{\triangleright}$, derived as $(1-\gamma/2)$ -quantiles of the probability distribution, $f(\tilde{y}|y)$, of the true value given the experimental result and the prior knowledge that the measurand is non-negative. They are calculated via the conditions:

$$P(\tilde{y} < y^{\triangleleft} \,|\, y) = \int_0^{y^{\triangleleft}} f(\tilde{y}|y)\, d\tilde{y} = \gamma/2 \tag{F.14}$$

$$P(\tilde{y} > y^{\triangleright} \,|\, y) = \int_{y^{\triangleright}}^{\infty} f(\tilde{y}|y)\, d\tilde{y} = \gamma/2 \tag{F.15}$$

This leads to the explicit equations:

$$y^{\triangleleft} = y - k_p\, u(y) \text{ with } p = \omega \cdot (1-\gamma/2) \tag{F.16}$$

$$y^{\triangleright} = y + k_q\, u(y) \text{ with } q = 1-\omega\gamma/2 \tag{F.17}$$

The parameter ω is given by

$$\omega = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{y/u(y)} \exp\left(-\frac{v^2}{2}\right) \mathrm{d}v = \Phi\left[y/u(y)\right] \tag{F.18}$$

If a non-zero effect is observed, i.e. $y > y^*$, the best estimate, $\hat{y}$, of the measurand (Figure F.4) can be calculated as the expectation of the probability distribution, $f(\tilde{y}|y)$, and the standard deviation of $\tilde{y}$ is the standard uncertainty, $u(\hat{y})$, associated with the best estimate, $\hat{y}$, of the measurand, Y:

$$u^2(\hat{y}) = \mathrm{Var}(\tilde{y}|y) \tag{F.19}$$

Using ω from Equation (F.18), the best estimate $\hat{y}$ is calculated (see Reference [38]) by

$$\hat{y} = \mathrm{E}(\tilde{y}|y) = y + \frac{u(y) \cdot \exp\left\{-y^2 \Big/ \left[2 \cdot u^2(y)\right]\right\}}{\omega\sqrt{2\pi}} \tag{F.20}$$

with the associated standard uncertainty, $u(\hat{y})$

$$u(\hat{y}) = \sqrt{u^2(y) - (\hat{y} - y) \cdot \hat{y}} \tag{F.21}$$

The following relationships $\hat{y} > y$ and $\hat{y} > 0$, as well as $u(\hat{y}) < u(y)$ are valid. For $y >> u(y)$ the approximations $\hat{y} = y$ and $u(\hat{y}) = u(y)$ are valid.

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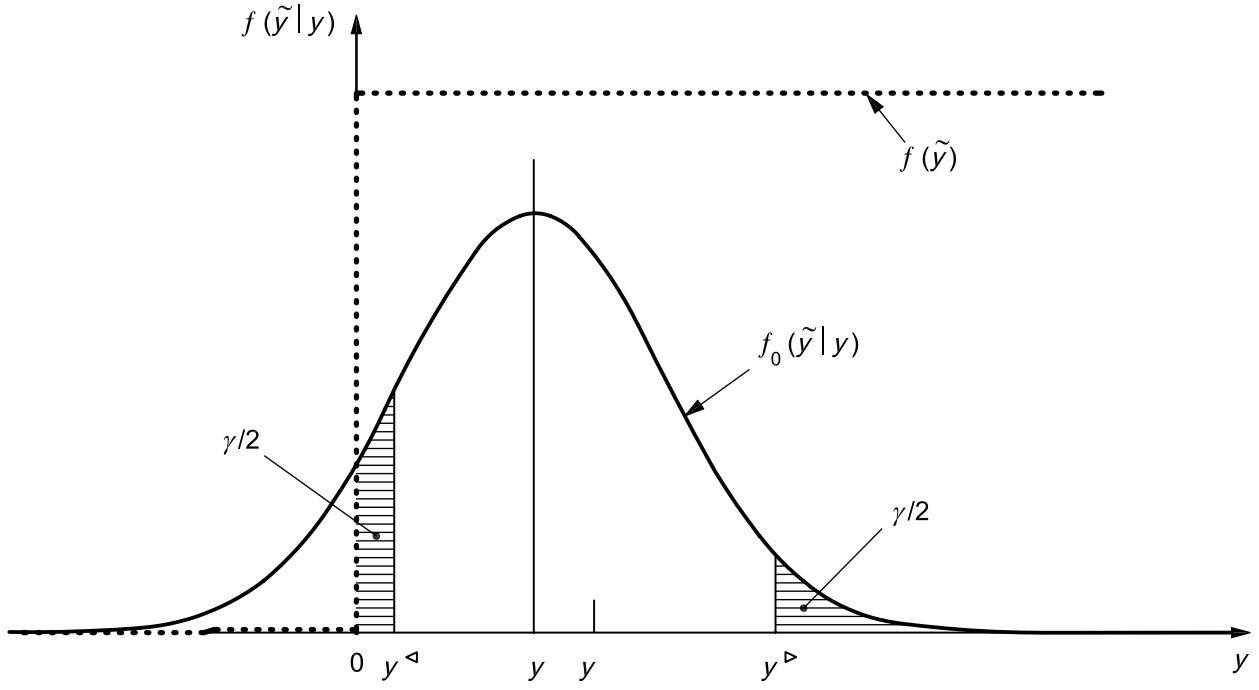

Key

$\tilde{y}$ true value of the measurand, Y

$f(\tilde{y}|\,y)$ probability distribution of the true value, $\tilde{y}$, of the measurand, Y, given the measured estimate, y

For the other symbols and curves, see the text.

Figure F.4 — Definition of the limits of the confidence interval and best estimate

The limits of the confidence interval are derived as $(1-\gamma/2)$-quantiles of the probability distribution, $f(\tilde{y}|\,y)$, of the true value given the experimental result and the a priori knowledge that the measurand is non-negative. The best estimate is the expectation value of this probability distribution, $f(\tilde{y}|\,y)$.

F.2.6 Assessment of an analytical technique

Having performed a measurement and an evaluation of the measurement according to ISO/IEC Guide 98-3 (see References [1, 2]), the performance of the analytical technique can be assessed in the following way:

A measured result shall be compared with the decision threshold calculated by means of Equation (F.11). If a result of the measurement, y, is larger than the decision threshold, y^*, one decides that a non-zero effect quantified by the measurand is observed and that the element or activity is present in the sample.

To check whether a measurement procedure is suitable for measuring the measurand, the calculated detection limit shall be compared with a specified guideline value, e.g. according to specified requirements on the sensitivity of the measurement procedure for scientific, legal or other reasons. The detection limit shall be calculated by means of Equation (F.13). If the detection limit thus determined is smaller than the guideline value, the procedure is suitable for the measurement, otherwise it is not.

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